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Workshop on Verification of Water Quality Models

Hydroscience, Inc.,
Westwood, NJ

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The U.S. Environmental Protection Agency sponsored a "National Workshop on the Verification of Water Quality Models" to evaluate the state-of-the-art of water quality modeling and make specific recommendations for the direction of future modeling efforts. Participants represented a broad cross-section of practitioners of water quality modeling in government, academia, industry, and private practice. The issues discussed during this workshop, which was held in West Point, N.Y., on 7-9 March 1979, were models in decision-making, model data bases, modeling framework and software validation, model parameter estimation, model verification, and models as projection tools. These topics were discussed by workshop participants who were organized into small groups, each of which discussed the state of the art of a specific branch of water quality modeling. Groups were divided into areas of wasteload generation, transport, salinity-TDS, dissolved oxygen-temperature, bacteria-virus, eutrophication, and hazardous substances.

Workshop findings were summarized by committee reporters and are presented in state-of-the-art reports. Workshop participants also prepared basic issue reports and technical support papers, all of which are included in this document.

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OF
WATER QUALITY MODELS

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FOREWORD

As environmental controls become more costly to implement and the penalties of judgment errors become more severe, environmental quality management requires more efficient analytical tools based on greater knowledge of the environmental phenomena to be managed. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Technology Development and Applications Branch develops management or engineering tools to help pollution control officials achieve water quality goals through watershed management.

Mathematical models are increasingly used in providing a technical basis for water quality management decisions and the formulation of environmental policies at all levels of government. Because of this increasing use and the increased interest on the part of scientists and engineers in modeling techniques, the U.S. EPA sponsored a workshop in which the latest information on the development and application of models to environmental decision-making was presented. This report presents the results of the workshop, which brought together a representative cross-section of water quality modeling experts from government, private organizations, and academia.

David W. Duttweiler
Director
Environmental Research Laboratory
Athens, Georgia

ABSTRACT

The U.S. Environmental Protection Agency sponsored a "National Workshop on the Verification of Water Quality Models" to evaluate the state-of-the-art of water quality modeling and make specific recommendations for the direction of future modeling efforts. Participants represented a broad cross-section of practitioners of water quality modeling in sections of government, academia, industry and private practice. The issues discussed during this workshop, which was held in West Point, N.Y., on 7-9 March 1979, were models in decision making, model data bases, modeling framework and software validation, model parameter estimation, model verification and models as projection tools. These issues were discussed by workshop participants who were organized into small groups, each of which discussed the state of the art of a specific branch of water quality modeling. Groups were divided into areas of wasteload generation, transport, salinity-TDS, dissolved oxygen-temperature, bacteria-virus, eutrophication and hazardous substances.

Workshop findings were summarized by committee reporters and are presented in state-of-the-art reports. Workshop participants also presented basic issue reports and technical support papers, all of which are included in this document.

This report was submitted in partial fulfillment of Contract No. 68-01-3872 by Hydroscience, Inc., under the sponsorship of the U.S. Environmental Protection Agency. This report covers the period from September 1979 to December 1979, and work was completed as of December 1979.

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SUMMARY*

Background

In the 50 years since the classical work of Streeter and Phelps, the use of mathematical models of water quality has grown extensively. In recent years, both advanced computer technology and increased USEPA support have combined to greatly increase the numbers of scientists and engineers using modeling techniques. At the present time, such techniques contribute to wastewater management decisions and the formulation of policy at local, state, regional and national levels.

Since their introduction, modeling techniques have grown in sophistication, complexity and in general use. A vast array of software is available for calculating input wastewater loads as well as water quality impacts. Mathematical models vary in their ability to simulate water quality variables, and in their levels of spatial, temporal and kinetic detail.

Because of the current use of mathematical modeling in providing a technical basis for many important decisions, the potential contributions in new decision areas, and because increasing numbers of people are using or applying models, the U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, Ga., sponsored a "National Workshop on the Verification of Water Quality Models."

Purposes

The workshop was organized to:

(1) examine current general capabilities and limitations of mathematical models

(2) identify methods of verifying model accuracy in specific situations

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(3) assess the reliability of decisions made on the basis of modeling results

(4) determine the needs and future directions that modeling efforts can most productively follow.

In addressing these concerns, the workshop brought together a representative cross section of participants from government, private and academic sectors who are experienced in the development and application of water quality models. The overall purpose of the workshop was to elicit from this cross section of model practitioners expressions of the present state of the art of model capabilities, credibility and utility and to suggest areas for improving model performance, verification and ability to respond to cogent water quality problems.

Format

A Workshop coordinating committee composed of the Workshop Co-chairmen (Thomas Barnwell, USEPA Environmental Research Laboratory, Athens, Georgia and Robert V. Thomann, Manhattan College), Workshop Coordinators and John P. St. John of Hydroscience, Inc., prepared invitations to selected individuals, formulated the Workshop agenda and program and prepared the Summary and Recommendations. The invited participants met on March 7-9, 1979 at the Hotel Thayer on the grounds of the U.S. Military Academy, West Point, N.Y. The workshop was coordinated by Hydroscience, Inc., Westwood, New Jersey.

On the first day of the workshop, all participants heard speakers address the basic issues of:

(1) Role of Models in Decision Making
(2) Data Base
(3) Time and Space Scales; Kinetic Detail; Cost Effectiveness
(4) Parameter Estimation
(5) Measures of Verification
(6) Use of Models as Projection Tools

On the second and third days of the workshops, invited participants were assigned to committees to discuss the above Issues as they relate to the use of models in the topical areas of:

(1) Wasteload Generation
(2) Transport
(3) Salinity/Total Dissolved Solids
(4) Dissolved Oxygen/Temperature
(5) Bacteria/Virus
(6) Eutrophication
(7) Hazardous Substances

All Committees then reported on the results of this discussion in two plenary sessions; one on the state-of-the-art and a second on recommendations.

In general, the draft Committee reports submitted by the Committee Chairman at the close of the Workshop shortly thereafter were compiled by Hydroscience in a standard format and sent out for review by Committee members. Subsequent comments were incorporated by Hydroscience and a final report resubmitted to the Committee Chairman for approval.

This publication therefore includes the papers presented by the authors on the six Basic Issues; summaries of Topical Committees discussions; and nineteen Technical Support Papers.

Present State of the Art

The following represents a summary of the principal conclusions reached by the Committees on Topical Areas in addressing the six Basic Issues of water quality verification.

Role of Models in Decision Making

A general consensus of the workshop participants was that mathematical modeling results of physical/chemical/biological processes along with other factors such as legal requirements, public opinion and economic considerations are used by decision makers in developing water quality plans. Although most administrators are usually well informed about decision making factors, it was recognized that modeling results can also be misused.

For example, some decision makers do not accept formal models as tools to be used in the decision making process but rather accept modeling results without question, especially when the results agree with the administrators' pre-conceived notions. In this light, the workshop noted that one of the modelers' functions is to keep the administrators informed on the strengths, weaknesses and limitations of the modeling results so that they can better understand the usefulness and reliability of model results. A strong responsibility therefore rests on the modeler to carefully explain and document the inherent assumptions so as not to "oversell" a model that promises more than it delivers.

In addition, workshop participants believed that transport, salinity/total dissolved solids (TDS), dissolved oxygen (D.O.)/temperature (Temp.), bacteria and eutrophication models are technically sound and when properly applied and verified, are capable of supporting water quality management decisions. At this time, members of the Wasteload Generation Committee concurred that the Non-Point Source (NPS) wasteload generation models are capable of planning level and guidance decisions but members questioned the accuracy of the models in their ability to test best management practices (BMPs) or alternative control effectiveness.

Finally, the members of the Hazardous Substances Committee indicated that hazardous substance models are not widely used in developing management plans.

In summary, committee members agreed that models are useful and necessary tools to be used as part of the decision making process by administrators. Members also encouraged the ongoing development of all model types especially the new technology wasteload generation and hazardous substance models.

Data Base

In order to perform a defensible water quality modeling study, Committee members acknowledge the need for extensive data bases. EPA presently sponsors and controls the nationwide computerized data handling and storage system known as STORET.

All topical committees agreed that as it presently stands STORET is often inadequate for modeling purposes. Workshop members believe that STORET and other generalized data bases contain large quantities of water quality monitoring data. These data are not always useful to modelers because monitoring data are generally not collected synoptically nor are the data specific enough for the individual modeling studies. In addition, there is a significant lack of spatial coverage of samples for individual water systems.

A general consensus of opinion was that good water quality data bases containing synoptically collected water quality data, input data, parameter rate data and detailed spatial coverage is necessary. Because these data are expensive to collect and specific to individual modeling studies, generalized data bases do not contain these data and are, therefore, not widely utilized for modeling studies.

Modeling Framework and Software Validation

Committee members noted that models for each of the topical areas can vary in complexity from simple spatial and temporal scales with simple mathematical solution techniques and basic kinetics to large complex models with long solution times and detailed kinetics. Members also concluded that model software is not always checked for accuracy and/or conservation of mass resulting in models that may not be numerically or scientifically accurate.

There was general concurrence that the complexity of models and detail of model subroutines are best analyzed at the start of an investigation. The resulting model detail also depends on project budget, complexity of the physical system, problems and questions to be answered, the timing of the project and the available technology. Members also agreed that, in general the simplest models and kinetic subroutines consistent with the problem context are the best approaches both in understanding model output and in conveying model results. Complexity in models should only be introduced where necessary.

Parameter Estimation

At present kinetic model parameters are estimated from special data collection programs, laboratory studies, literature reviews and calibration procedures. Strict reliance on literature kinetic rates was recognized as a poor modeling practice unless the system is fairly insensitive to changes in the kinetic rates. Better modeling practices rely on special site specific field studies and model calibrations to estimate parameter kinetic rates, using the literature values as guidelines. Sensitivity Analysis is recommended as a valuable adjunct to the parameter estimation process.

Measures of Verification

Workshop members generally agreed that models are first calibrated to define system kinetic parameters and then verified to provide a measure of confidence in the model. For adequate verification, the computed model results are compared to a set of water quality data other than the calibration data set. In the second comparison, system kinetics remain constant except for changes which are functions of temperature, salinity, flow or other system parameters.

Members also agreed that statistical measures of verification are available but are not widely used. Present verifications are based on graphical comparisons between computed model results and observed data, with the engineer's judgment serving as the qualitative measure of verification. This method of verification, although qualitative in nature, remains a solid engineering practice. However, quantitative verification techniques were recognized by committee members as useful tools for future studies. There was general agreement that no one statistical technique for verification should be promulgated.

Use of Models as Projection Tools

The purpose of water quality models is to aid in understanding the cause and effect relationships between wastewater inputs and water quality impacts, so that treatment alternatives can be evaluated as they affect future water quality. Workshop members concurred that except for wastewater generation models, all other models, when properly verified, adequately predict incremental changes in water quality in the evaluation of alternatives. Members also agreed that almost no post audit surveys have been conducted to date to check the results of water quality projections. Therefore, the accuracy of model projections can only be related to the quality of the model verification.

RECOMMENDATIONS*

The following recommendations are summaries of recommendations made by the workshop members. Detailed recommendations for future development efforts and modeling practices follow each of the committee reports.

1. The workshop members encourage better coordination and communication between the modeler and the decision maker, in order to increase the understanding and credibility of models.

2. The workshop members recommend that modelers should be involved in data collection efforts and planning efforts to improve the data available for modeling studies. A comprehensive high quality data base for purposes of model testing, verification, and improvement should be established. This should include high quality synoptic data bases obtained from selected water bodies including "impoundments", selected river and estuarine systems and controlled field experiments.

3. The workshop members encourage continued and expanded software code review and internal automated checks for the purpose of proper computer program validation.

4. The workshop members encourage expansion of laboratory studies and special field studies to further develop parameter kinetics. This is recommended for all areas of modeling especially for hazardous substance modeling.

5. The members encourage the use of statistical verification techniques. However, no single technique is recommended nor should statistical techniques be used to supercede engineering judgment. Sensitivity analysis is recommended as a key to verification and parameter estimation.

6. The Eutrophication and DO/Temp Committees recommend that resources be allocated for post audit data collection programs and subsequent model studies to verify previous model projections.

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*Prepared by Hydroscience, Inc.

ROLE OF MODELS IN DECISION MAKING

by

John T. Marlar[1] and James S. Kutzman[2]

There is an increasing awareness of the role of mathematical modeling of water quality impacts in arriving at informed decisions regarding wastewater management. This increasing awareness covers a wide spectrum which ranges from complete skepticism to total faith. The purpose of this paper is to examine the use of outputs from such models and how such outputs are used in conjunction with other factors to arrive at defensible decisions. In order to perform this examination, a recent case involving mathematical modeling and how the results were used will be presented. This case illustrates how model results can be used in arriving at decisions and also offers several germane points that are essential if model outputs are to be useful in reaching decisions.

The South River is a small river whose headwaters originate near the City of Atlanta. The river is tributary to Lake Jackson and is approximately 60 miles in length. The river receives treated wastewater from several major municipal treatment facilities. In 1972, the following effluent limitations were established for wastewater dischargers to the South River:

BOD_5 = 10 mg/l

NH_3-N = 2 mg/l

D.O. = 6 mg/l

Phosphorus = 1 mg/l

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[1] Chief, Technical Support Branch, Water Division, USEPA, Region IV; presented paper.

[2] Chief, Applied Technology Section, Technical Support Branch, USEPA, Region IV.

The oxygen demanding constituent limitations were based on a mathematical model of the river and the phosphorus limit was based on a water quality analysis of the nutrient components in Lake Jackson. Using these effluent limitations as a basis, facility plans were prepared for the areas and the actual design work was completed. The City of Atlanta determined it would be cost-effective to remove its discharges from the river and transfer them to an adjacent basin. DeKalb County decided to upgrade existing facilities to meet the effluent limitations. The planning and design work took approximately 5 years to complete with the resulting total construction cost estimated at $150 million. In March 1978, after completion of the design of advanced waste treatment facilities, DeKalb County requested that the effluent limitations be relaxed back to secondary treatment. The request was made through their congressional representative. As a result of this request, EPA Headquarters in Washington conducted an independent investigation into the technical basis supporting the effluent limitations. In addition to this, DeKalb County hired its own consultant to likewise investigate and examine the basis. The review by EPA Headquarters indicated there was a firm technical basis for the effluent limitations and that the limitations were supportable. The consultant hired by DeKalb County concluded there was absolutely *no* basis for the effluent limitations. This conclusion was refuted by the regional office of EPA in Atlanta. Faced with an apparent total disagreement between "experts", the county hired yet another consultant to review the first consultant's work and the EPA review of the project. This last consultant concluded that there probably was a sufficient basis for the effluent limitations or at least that the county would not be able to easily prove their case. As a result of these reviews, DeKalb County is presently proceeding with the construction of most of the facilities designed to produce the original effluent limitations established in 1972. Much of the controversy appeared in the media and generated a great deal of local interest. This example of the development and use of the effluent limitations on the South River is abbreviated with many of the details omitted from this paper. Copies of the review reports mentioned above are available for your further consideration, i.e., references (1), (2), (3) and (4).

The example used here illustrates several points germane to the use of models in making wastewater management decisions. These points should be kept in mind when future decisions are made based on model outputs.

1. The basis used in establishing the effluent limitations was technically strong and defensible. The effluent limitations for BOD_5, NH_3-N and dissolved oxygen were based on a dissolved oxygen model of the river. The input parameters to the model were based on intensive stream surveys, supplemented by other data collection efforts. The reaeration rate of the river was measured in the field using the gas

tracer technique developed by Dr. E. Tsivoglou. The phosphorus limitation was based on a study of the nutrient budget or input-output approach of nitrogen and phosphorus loadings to Lake Jackson. This approach has been compared to more sophisticated "eco modeling" approaches and was found to yield similar results, reference (5). Further studies done in 1974 and 1977 reexamined the phosphorus limitation in light of new techniques and a changing situation regarding the wastewater discharges to the lake. The conclusion of these studies was that the lake would be phosphorus limited and that by implementing the 1 mg/l limitation on phosphorus, the eutrophication problems in the lake would be arrested.

The effluent limitations were not based on an arbitrary policy or decision but rather were based on a firm technical foundation. The model outputs were based on modeling efforts that were logical, reasonably well documented, and defensible. In many cases model outputs do not have strong foundations. If a decision maker is going to use model outputs in arriving at wastewater management decisions, the technical personnel should provide as good a technical basis as can be prepared. Such personnel should also be able to advise the decision maker as to whether or not the modeling work is strong or weak. Frequently, technical types are apprehensive about indicating the weaknesses or strengths of modeling work. It is important that any decision maker have an objective appraisal regarding how good or bad the supporting modeling work appears to be. In the South River case, the decision makers were advised that the modeling work was good enough to support the limitations. In other cases, the advice to the decision maker has been that the modeling work was not adequate to support the conclusions and that the outputs should not be the sole basis of the decision. It is essential that the technical personnel provide not only the model output but an objective evaluation as to the credibility of the work supporting those outputs.

2. It is appropriate for technical personnel to advise the designated decision maker as to the model outputs and the merits of the outputs. These outputs are one contributing factor but not often the sole factor. Both the technical personnel and the decision maker should realize this. In many cases, either too much or too little reliance is placed on model results. A proper balance of all significant factors must be maintained.

3. There are many factors which can be used in conjunction with model results in arriving at a wastewater management decision. In the South River case, two separate major decisions were made. One was made in 1972 and the other

was made in 1978. The decision in 1972 was to require municipal wastewater dischargers to meet the prescribed level of treatment. Aside from the model outputs, other factors were considered in the decision. Local environmental groups expressed considerable interest in improving the quality of the river. Residents of the Lake Jackson area were extremely concerned about the deteriorating water quality of the lake. There was vocal public support for any efforts to improve the river and lake. Another factor was that local governmental entities were interested in expanding their waste treatment facilities and wanted to be eligible to receive federal funding for the construction of the facilities.

In 1978, the decision was whether to continue to require DeKalb County to meet the established effluent limitations. There were different factors to consider in making this decision than there were in making the 1972 decision. Although the technical basis for the model results was improved, the political factors had radically changed. The major political entity involved no longer accepted the effluent limitations. DeKalb County attempted to utilize means other than direct conversation with the State and EPA to delay or eliminate the limits. The tone and direction of EPA concerning advanced waste treatment projects had changed. Questions were being raised nationally concerning the need for higher levels of treatment. The third additional factor was the precedent factor. There were many other communities observing what decision would be reached and how they could use it. It should be remembered that the City of Atlanta had chosen to remove their discharges from the basin. The decision was based in part on the original effluent limitations. Any change in the effluent limitations for DeKalb County would create uncertainities over the decision made by the city. Another factor considered was the federal funding issue. Grants had been awarded to DeKalb County for the construction costs of facilities designed to meet the original effluent limitations. If the effluent limitations were changed, the possibility existed that the funds would be withdrawn from DeKalb County because the facilities would have to be redesigned. The last factor considered was that the plants could be given permits that would contain seasonal limitations. This would afford the county some operational cost savings and still attain water quality goals.

The above factors are the type that decision makers must consider in addition to the technical model outputs. Each situation will have its own set of additional factors.

4. The level of technical evaluation to support any modeling outputs should reflect the magnitude of the decision being made and the complexity of the water system being affected.

In the case of the South River, the evaluation was reasonably extensive which was important because the resulting cost of the final construction of the needed facilities was approximately $150 million. Another aspect of this point is that the approach selected should fit the situation. For example, the model selected should apply to the type of situation that is being examined. It is often not necessary to develop a new model but rather to apply an existing model with adequate data. In the case of South River a steady state, one dimensional dissolved oxygen model was utilized. It was not necessary to utilize a more sophisticated model. In determining the phosphorus limitation, it was necessary to modify the Vollenweider approach to approximate actual conditions observed in Georgia lakes. This modification is the type of change that personnel doing water quality analyses should be aware of. It is not enough to merely put numbers into a program and obtain results. It is necessary that the personnel be able to analyze, interpret and understand what a model's output means.

The four points mentioned above are by no means an all encompassing list. They do represent points that all individuals who are involved in modeling should give consideration to. The most important point however in the administrator's use of model output is the credibility of the technical personnel providing these outputs. Technical personnel must be able to give a decision maker a clear, objective appraisal of the merits of the outputs.

It is also necessary that the technical personnel understand that they are part of a decision making process and should not be expected to make the decisions. They should be an integral part of the process and should contribute to the decision, but it is equally important that decisions be made at the proper level.

REFERENCES

1. Review of Advanced Wastewater Treatment Works Proposed for DeKalb County, Georgia, Office of Water Programs Operation, U.S.E.P.A., November 7, 1978.

2. Analysis of AWT Effluent Limits for DeKalb County, Georgia, Jerome Horowitz and Larry Bazel, October 5, 1978.

3. Review of Report Entitled "Analysis of AWT Effluent Limits for DeKalb County, Georgia" prepared by Jerome Horowitz and Associates; Technical Support Branch, Water Division, EPA Region IV, November 7, 1978.

4. Letter from Dr. Ernest C. Tsivoglou to Walter B. Russell, Jr., Chairman of DeKalb County Commission, December 1, 1978.

5. Comparison of Eutrophication Models, John S. Tapp, U.S.E.P.A., Region IV, May 1976.

STORET: A DATA BASE FOR MODELS

by

Phillip L. Taylor[1]

One of the important topics before this workshop is the data base used by modelers. The data base is not all in one place and in many instances modelers are familiar with the situation of going to a number of sources to obtain data needed in the development of a model. Obtaining data such as time-of-travel, geometry, streamflow, or rainfall may involve contacting EPA, U.S. Geological Survey (USGS), Corps of Engineers (COE), or National Oceanic and Atmospheric Administration (NOAA). My topic today is EPA's data system - STORET - and I hope to shed some light on how it can be used by modelers.

For the sake of discussion, modeling is divided into three categories related to the geographic size of the area modeled and the type of data needed for the model. At one end of the spectrum are wasteload allocation models and at the other end are macro models of whole river systems. Between these are models for relatively large systems such as the Great Lakes or multi-county non-point source areas. There are many situations where STORET has data for a model category. A quick review of the data system covers types of data available, data sources, some of the analysis routines, and examples in which the data base was used in modeling.

The STORET system in its operation over the past 15 years has been used by many Federal, State and local monitoring programs which have collected and placed in the data base 50 million monitoring observations for 200,000 surface water sampling locations. These data are entered into the system on a daily basis by more than 225 computer terminals in 120 cities with master system updates each weekend.

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[1] Monitoring and Data Support Division, USEPA, Washington, D.C.

One of the major STORET data sources is the US Geological Survey. All of the water quality data collected by USGS is stored in WATSTORE for USGS purposes and it is transferred monthly to STORET for purposes of dissemination to other agencies and the public. Additionally, EPA periodically receives streamflow data tapes from USGS and STORET maintains the supporting software for its use. EPA and USGS have an interagency agreement for sharing these data, and another agreement with the Survey includes EPA's participation in the National Water Data Exchange (NAWDEX). As part of this latter agreement, STORET is indexed annually to assist NAWDEX referral services.

The Corps of Engineers, Bureau of Reclamation, TVA and U.S. Forest Service are important sources of STORET monitoring data for many streams, lakes and reservoirs associated with their areas of responsibilities. Data throughout the Great Lakes is provided by the International Joint Commission (IJC) through cooperative Canadian and U.S. programs.

States provide data to STORET from their ambient monitoring program. The principal guidance document, entitled the Basic Water Monitoring Program (BWMP) emphasizes the need for intensive surveys to be done in priority basins at least once every five years for developing wasteload allocations, setting water quality standards and assessing conditions in those basins. This activity, while serving State purposes, will make more data available to modelers for a wide variety of purposes.

EPA has several monitoring programs which generate various types of water quality data. The Regions and Headquarters provide priority pollutant data from ambient, fish and sediment samples. Effluent data are available from an increasing number of facility (both industrial and POTW) surveys. Regional data from on-going fate studies on toxic pollutants will be used for large scale modeling, but may also be of value to WLA modeling. Data in STORET from other studies, such as lake eutrophication surveys and Section 208 non-point source studies, should be useful in developing models of intermediate scale.

All of these many sources of data have collectively provided a very large data base, only part of which is of interest to this workshop. Table 1 shows the overall abundance of data in STORET in various topical areas. Shaded maps, such as Figure 1, are available for each topical area to show the geographic distribution of these data and to help investigators determine if needed data are available in the general location under study.

Data can be retrieved by station, basin, county, or irregular area (polygon). Examples for some of the STORET outputs are data inventories for each monitoring station, raw data listings, statistical summaries, computed daily stream loadings,

TABLE 1

STORET DATA AVAILABILITY
FOR
TOPICAL PARAMETERS

Topical Parameter	All Years Number of Observation (millions)	1975 Number of Observations (millions)	1975 Number of Stations (thousands)
Temperature	3.06	.295	29.9
Turbidity	.90	.096	12.2
Color	.54	.054	8.1
Conductivity	1.66	.143	22.1
Dissolved Oxy.	1.87	.199	20.4
TDS	0.74	.057	3.9
Chlorides	1.85	.094	17.2
Sulfate	.89	.061	13.2
Nitrogen-Total	.11	.021	4.4
-Organ.	.23	.028	5.7
-Ammonia	.77	.099	16.8
-Kjeldahl	.42	.086	11.9
Phosphorus-Tot.	.82	.117	19.6
Chlorophyll-A	.04	.006	0.8
Algae-Total	.06	.003	0.9
Coliforms - Total	.78	.046	7.2
- Fecal	.61	.107	14.9
DDT	.03	.005	1.7
Dieldrin	.03	.005	1.9
PCB-Total	.01	.003	.9
Chromium-Total	.14	.024	7.1
Mercury-Total	.13	.001	6.6

Reproduced from best available copy.

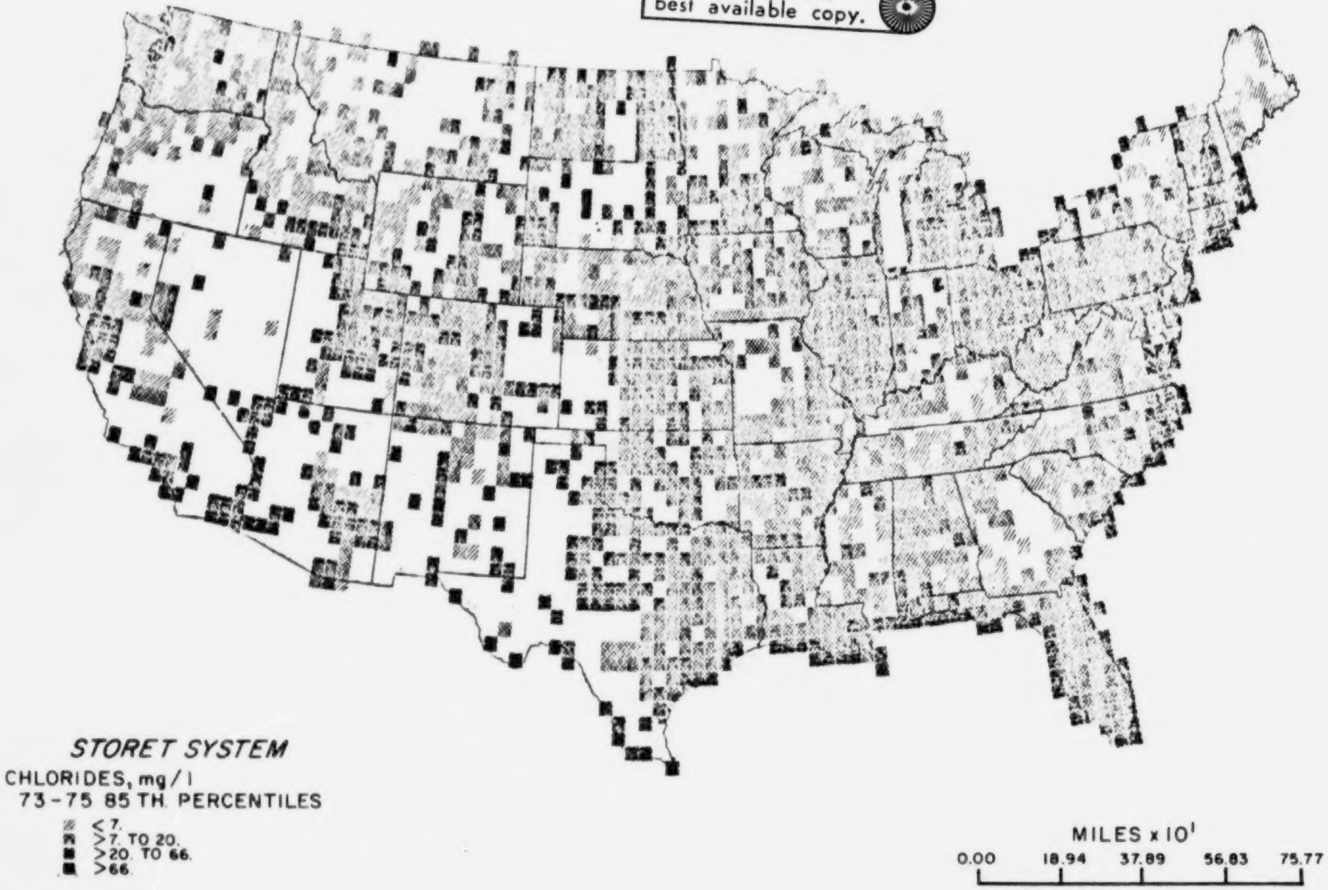

STORET SYSTEM
CHLORIDES, mg/l
73-75 85 TH. PERCENTILES
<7.
>7. TO 20.
>20. TO 66.
>66.
MILES x 10¹
0.00
18.94
37.89
56.83
75.77

FIGURE I. DATA AVAILABILITY, CHLORIDES

river profiles or water quality mapping. The STORET files can be interfaced with EPA software, system software, such as SAS, BMD, or with user supplied software. The STORET software was developed to meet specific user needs, including comparing water quality with standards, analyzing water quality trends, determining water quality improvement related to enforcement actions, or assisting in the general distribution of water quality data. If modelers identify additional requirements, STORET management would be able to include such requirements in future system development plans, both in terms of data acquisition and software for retrievals and displays most meaningful to modelers.

The STORET data base is just starting to receive a significant increase in intensive survey data from States, and EPA has proceeded to provide some special system capabilities. It is expected that this first step will be important in providing stream and effluent data for modeling purposes. The Basic Water Monitoring Program (BWMP) defines State water monitoring responsibilities, and calls for a shift toward more intensive surveys and away from excessive long term fixed station activities. The BWMP emphasizes the need to acquire excellent data in the intensive surveys for determining effluent limits for water quality based permits. These surveys will be important in developing cost effective plans for advanced waste treatment (AWT), advanced secondary treatment (AST) and treatment in excess of best available treatment (BAT). It is important that the decisions, locally and nationally, for higher degrees of treatment be based on sound data, because of the large economic and environmental implications associated with possible mistakes in this area.

Intensive survey data will be stored in STORET by the States and they can use the system as an analytical tool to help summarize and interpret survey data. The completion of a survey abstract (Figure 2) is a first step for storing intensive survey data. These abstracts will be used to assist in coding, storing and retrieving the survey data. Suggestions to help make the abstract better meet modelers' needs, both now and in the future, can lead to a STORET capability which will truly be of significant value in modeling activities.

The STORET analytical and display capabilities for open water data have potential value for linking data from separate cruises and near shore sampling together in a manner which can be compared with model outputs. These techniques can handle large amounts of data for many spatial and temporal situations. Data from Saginaw Bay in Lake Huron will help to indicate some conceptual uses of the data base.

The EPA Large Lakes Research Station at Grosse Ile, Michigan used Storet retrievals of raw data and contour plots (Figure 3) for Saginaw Bay to correlate with a LANDSAT imagery

FIGURE 2

INTENSIVE SURVEY ABSTRACT

Responsible Office ____________________ Person ________________

Phone ________________

Segment ID ____
(name of principal stream or water body)

Brief Description of Survey ________________________________
____

Location of Survey ____
(L/L polygon)

Parameters Measured

P =

P =

P =

etc.

Station Storage Data
or
Station Pointer Data

Agency/Station	Station Order	Lat/Long	State	Co	Type	Name	RMI (yes/no)
A= S=	Path I Path II Path III Path IV						
A= S=							
A= S=							

FIGURE 2
(Continued)
CHECK-OFF LIST

(1) Survey Purposes

Reconnaissance
Problem assessment
Model calibration/verification
Wasteload allocation
Municipal permits
Industrial permits
Other

(2) Sources/Problems

Storm or combined sewer
Non-point source agriculture
Non-point source silviculture
Non-point source urban
Lake eutrophication
Thermal
Stratification
Land disposal
Municipal
Industrial
Power
Irrigation
Other

(3) Land Uses - Non-point Sources

Residential
Office/shopping
Industrial
Agricultural
Homogeneous
Other

(4) Water Uses

Drinking water
Aquatic life
Sports fish
Commercial fish/shellfish
Recreation
Irrigation
Industrial supply

(5) Water Body Types

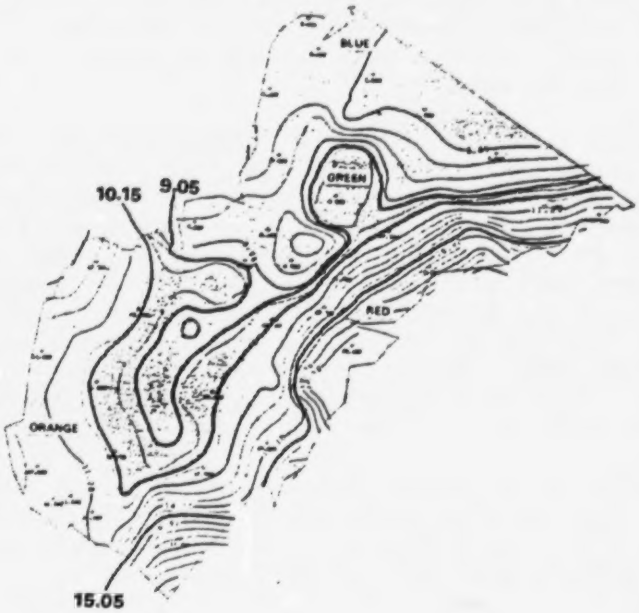
Stream
Lake
Impoundment
Estuary
Bay
Ocean
Swamp
Groundwater
Other

(6) Sample Types

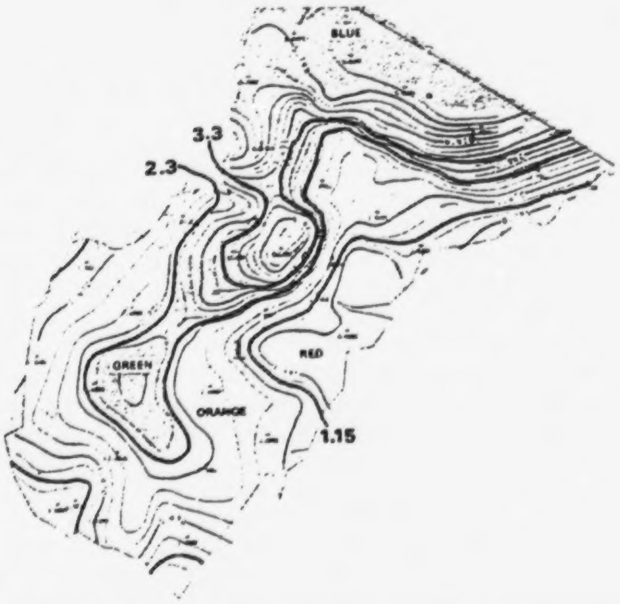
Ambient Water
Sediment
Fish
Rainfall
Precipitation
Streamflow
Point source
Raw water supply
Washoff
Other

(7) Parameter Groups

Physical
Biological
Bacteriological
Nutrients
Solids
Metals
Pesticides
Trace Organics
Other


BLUE
GREEN
10.15
9.05
RED
ORANGE
15.05

MACHINE CONTOURED CHLORIDE DATA,
33 STATIONS, JULY 29-31, 1975


BLUE
3.3
2.3
GREEN
RED
ORANGE
1.15

MACHINE CONTOURED SECCHI DEPTH DATA,
33 STATIONS, JULY 29-31, 1975

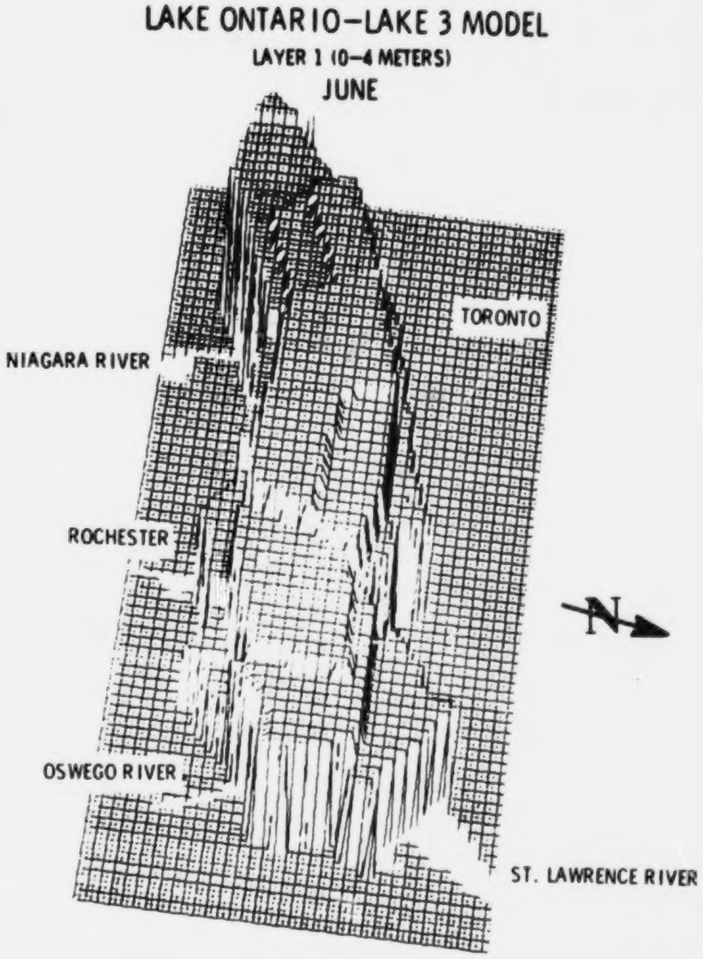
FIGURE 3. SAGINAW BAY CONTOUR PLOTS (STORET)

PRODUCTION OF A WATER QUALITY MAP OF SAGINAW BAY BY COMPUTER PROCESSING OF LANDSAT-2 DATA, BENDIX AEROSPACE SYSTEMS DIVISION project. The project objective was to investigate new surveillance and analysis techniques which were helpful in determining locations and relative magnitudes of water quality gradients in large bodies of water.

Another example of using STORET for open water analysis involved IFYGL data for Lake Ontario. One model output (Figure 4) was compared with two and three-dimensional plots (Figures 5 and 6) generated by STORET using IFYGL data in the system to help interpret the model results. One point of interest to the modelers was that these plots show irregular chlorophyll levels occurring along the shoreline particularly near Rochester and Oswego with some noticeable spikes which probably were attributable to algal blooms. These secondary factors should be taken into consideration when comparing the outputs of a model with actual ambient data.

An area of interest for all data users has been the quality of data. In January 1978, QA/QC began receiving high level attention when the Administrator established a select group, The Blue Ribbon Monitoring Committee, to review EPA's monitoring and data programs. The Committee was concerned with improving data quality associated with sampling, instrumentation, analytical methods, data processing, and other methodologies. Because of new priorities on toxics, several protocols for field sampling and lab analysis have been improved to provide greater assurance that the toxics monitoring data are reliable. Paralleling the field and lab work, STORET is keeping pace with new requirements through adjustments to accomodate QA and QC codes, multi-media data and parameters to cover the many organics being found with GC/MS instrumentation.

EPA Headquarters is currently conducting a program to evaluate exposure and subsequent risk from the presence of toxic pollutants in the water environment. This program is using the EXAMS (Exposure Analyses Modeling System) model developed by EPA's Environmental Laboratory in Athens, Georgia to model 114 organic compounds on the list of 129 priority pollutants. EXAMS is a multicomponent kinetic model that synthesizes environmental fate and transport processes for a specific set of environmental conditions. The Headquarters program is in the process of developing various rate coefficients needed to run the model. The model's use of physical, chemical and biological fate processes are based on the results of literature reviews and laboratory studies. Data from Regional surveillance and analysis field studies on stream segments will help to better determine rate coefficients. The concept of stream and river reaches will be used later in the model so that fate evaluations can be made for actual waterways. This approach depends on the use of STORET to provide data which is available for many miles of waters and computerized stream reaches. In many instances these



LAKE ONTARIO–LAKE 3 MODEL
LAYER 1 (0–4 METERS)
JUNE

PHYTOPLANKTON CHLOROPHYLL 'a' MAXIMUM, 8.2 μg/l

FIGURE 4. THREE DIMENSIONAL PLOT OF PHYTOPLANKTON CHLOROPHYLL CALCULATED FROM LAKE 3 MODEL–JUNE, 0–4 METERS.

THOMANN, et. al. DEVELOPMENT AND VERIFICATION, I. MODEL
MATHEMATICAL MODELING OF PHYTOPLANKTON IN LAKE ONTARIO
1976. (EPA-660/3-76-065)

LAKE ONTARIO CHLOROPHYLL 'a', $\mu g/l$ PARM 32210

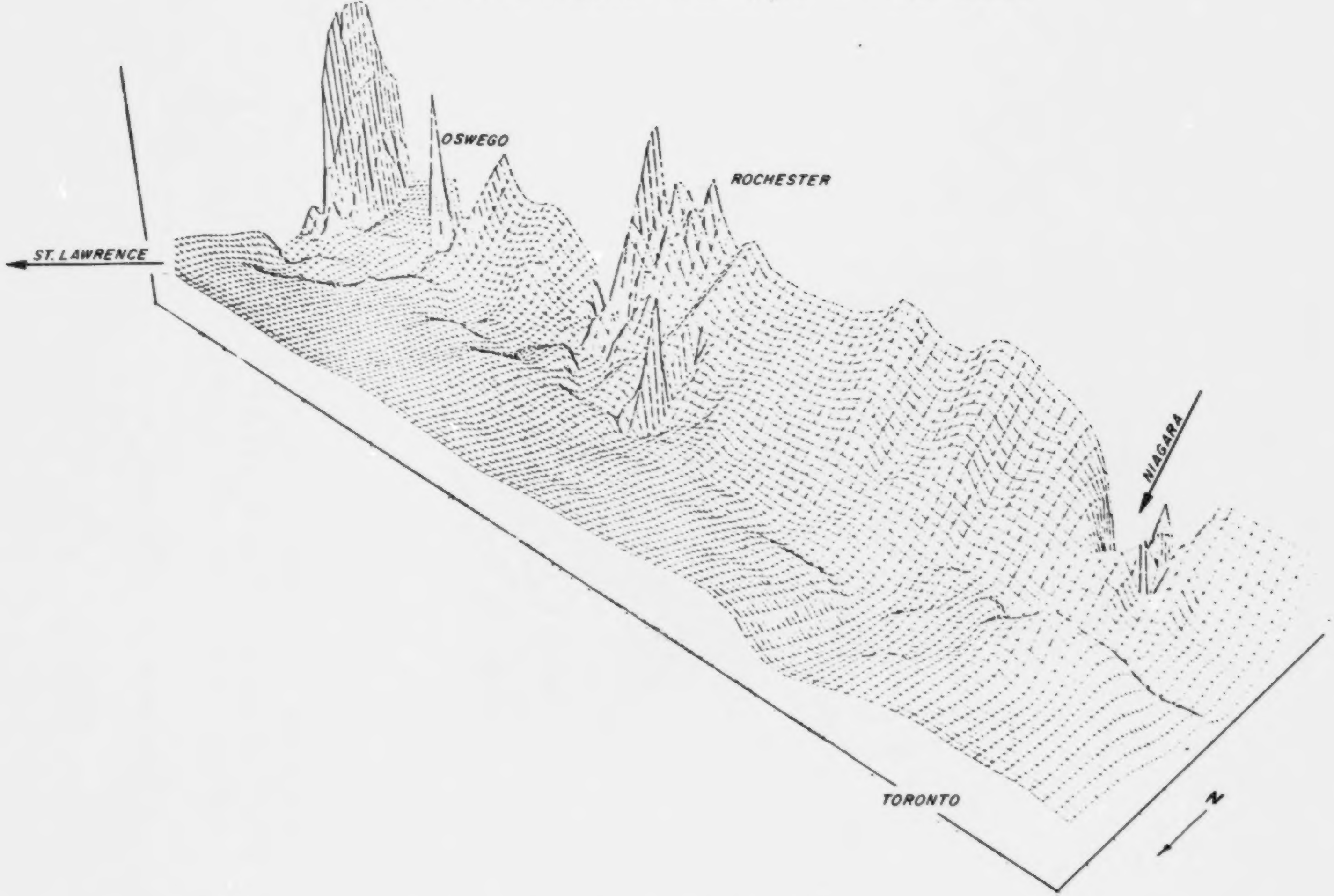


FIGURE 5. LAKE ONTARIO–CHLOROPHYLL 'a' (ALL DATA), 1972 MONITORING DATA FROM STORET

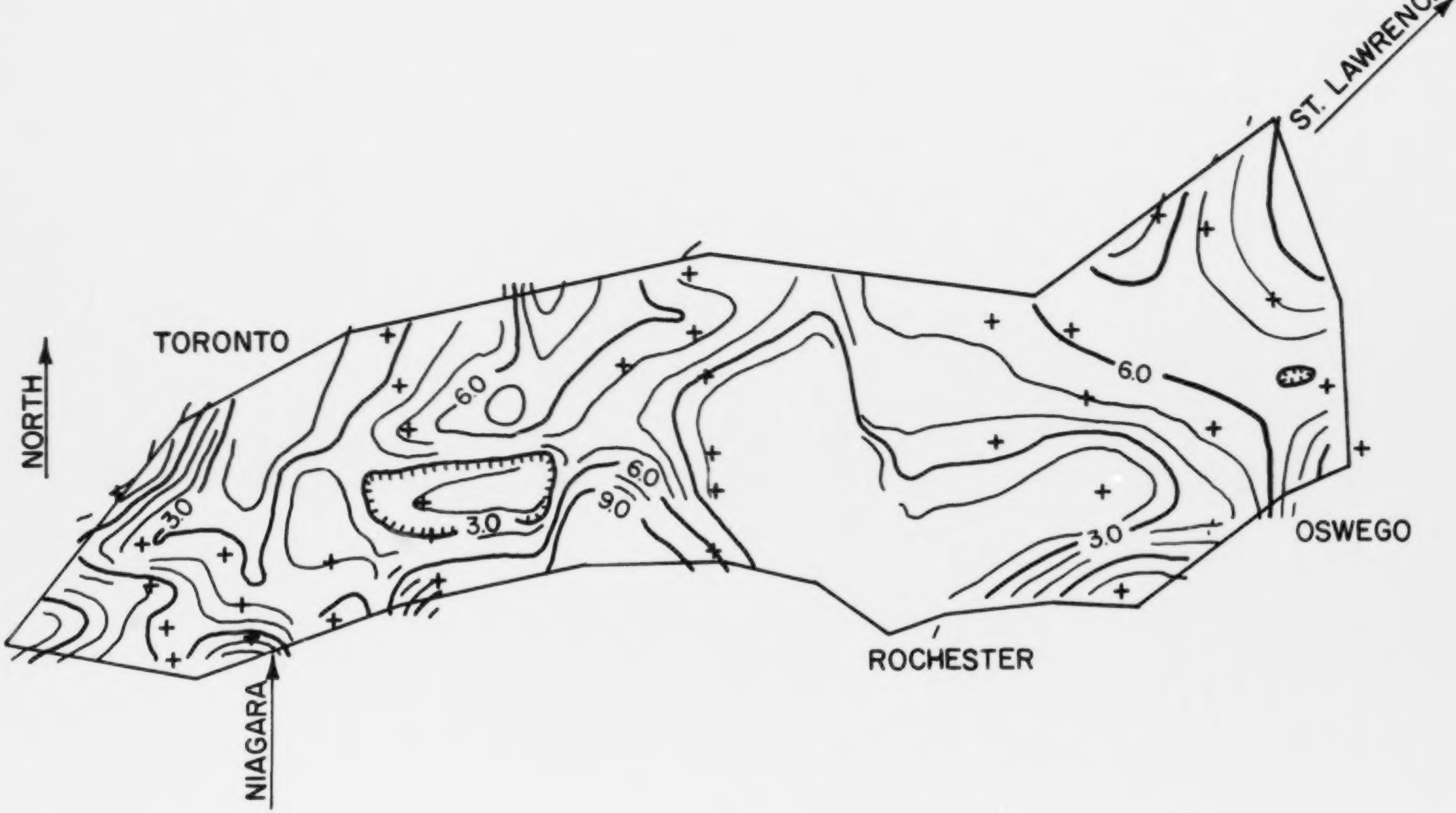

NORTH
TORONTO
ST. LAWRENCE
OSWEGO
ROCHESTER
NIAGARA
6.0
3.0
9.0

FIGURE 6-LAKE ONTARIO-CHLOROPHYLL 'a' (0-4 METERS). JUNE 1972 MONITORING DATA FROM STORET

data will be used to enhance or replace simulated data from models.

Rivers and streams of the United States are being digitized by EPA for a data base called the Reach File. It will include approximately 50,000 stream reaches, representing one seventh of the country's streams. The file will be a framework for simulated routing of streamflow and pollutants through the Nation's river systems. One of the first uses of the file will be to better describe stream conditions used in the EXAMS model so that fate evaluation can be made for an actual river or stream reach using existing data rather than simulating all conditions.

In conclusion it is clear that limited use has been made of STORET as a data source for modelers. Some modelers do use it to store and sift through data they gathered for wasteload allocation efforts. This need is increasing and the means for handling the associated data should be improved. On a larger scale, STORET toxics data and the Reach File will play an important role in modeling whole river systems. These efforts will be accompanied by strengthened activities for improving data quality.

MODELING FRAMEWORK & SOFTWARE VALIDATION

by

John P. Lawler[1]

I. MODEL FRAMEWORK - ELEMENTS

- Time Variable or Steady State
- One, Two or Three Dimensional
- Completely Mixed, Plug Flow, Partially Mixed
- Time Averaged, Space Averaged
- Deterministic, Stochastic
- Empirical, Conceptual (Mechanism)
- Linear, Non-linear
- First-order, Zero-order, Michaelis-Menton
- Single Species, Multi-species, Community
- Population vs Ecological Level
- Hydrodynamic, Mass Transport, Energy Flow
- Physical, Chemical, Biological Kinetics & Transport
- Combinations of many of the above

II. GUIDELINES FOR ELEMENT SELECTION - BROADER THOUGHTS SOMETIMES LOST

Delineation of the Problem vs Mechanics of Solution: Too often, the modeler takes a given outline of the problem as *the given*; i.e., a cast-in-concrete perception which only requires a solution into which he is only too glad to plunge. Immediately there follows a careful, or sometimes not so careful, sorting of model elements, such as those described above, and an eventual choice of a model framework and solution technique.

Some thoughts are offered toward broader views on which the modeler might well reflect on prior to taking the plunge. It has been my experience that these and like considerations eventually surface in most modeling efforts. The trick, I believe, is to start here - not find out after six months or two years or ten year of study effort - and associated dollars, that a recasting must take place, which could have been avoided with a little more foresight. Of course, hindsight is supposed to be better than foresight, but as modelers, our predictions are supposed to eventually verify. I submit the better the early broad-base thinking, the better will be our simulation of "the problem", regardless of the eventual choice of model framework and solution nitty-gritty.

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[1] Partner, Lawler, Matusky & Skelly Engineers, Pearl River, New York.

Narrow vs Broad Scope: Where should emphasis be placed - on modeling the water quality changes and improvements to be expected in the presence of upgraded point source treatment, or on the total picture, including non-point source pollution? Are our priorities properly placed if we ever refine our ability to simulate water quality changes accruing from water supply development and point source treatment, and forget that introduction of these utilities change the growth pattern and growth rate of a community? Positive (or negative, depending on your point of view) feedback, to be sure!

Single vs Multiple Effects: Where should emphasis be placed - on concerning ourselves with the hypothetical impact of a single aspect of a single industry on a single species of fish, or on the multiplicity of interrelated phenomena that together make up the real world condition, good or bad, of our nation's waterways?

No Action vs Alternative Actions: Shall we stifle needed projects because, by comparison to the "no action" alternative, they are viewed as producing unacceptable impacts or levels of risk. Here we are not addressing the valid "no action" alternative, but rather the comparison to the absence of any project in the past, in situations where some project must proceed, or already exists.

Zero Discharge vs Acceptable Levels of Water Quality Change: Toxic substances are now a fact of life. Shall we wring our hands in despair, as the "carcinogen of the week" is announced, or shall we work toward an ever better understanding of the kinetics, transport and distribution of these substances in our air, land and water, at the same time others are working toward a similar ever better understanding of their impact on man? This is an area, I believe, where sophistication and refinement of today's modeling technology, often overused in many applications, will be tested. Substantial advances in many of the elements listed above will be necessary.

The Planner vs the Modeler: The theme of each of the foregoing thoughts revolves around the responsibility of all engaged in delineating a problem and framing its solution to ensure the problem is properly defined and fully described before proceeding to simulate the particular real-world phenomena. Too often, the modeler is satisfied to take his direction from the planner, the administrator, the regulator, without recognizing the role he can play in defining and guiding that direction. After all, if he is charged with a real world simulation, then he ought have insights that others may not have. At the very least, he should train himself to think broadly, so that he contributes at the time when broad thinking is required.

III. MODEL VALIDATION

Model validation or "acceptance testing" entails verifying that the working model does indeed represent the system it has been constructed to represent. Although this step includes "program debugging," it is by no means limited by this procedure. During this step, the "working" model is compared with "known" analytical or numerical solutions similar to the current system. This is achieved by "degenerating" the "working" model to simpler systems with accepted solutions, usually by the judicious selection of test data.

For example, a dynamic model must eventually reach a steady state, given repetitive input and boundary conditions. The results of the "working" model can be compared with a steady-state solution with the same test data; the comparison is made after sufficient time has elapsed for the "working" model to damp out the transient behavior resulting from the initial conditions.

A model developed with space variable parameters, e.g. variable cross-sectional areas, can be compared to an analytical or numerical solution developed for constant cross-sectional areas by the use of constant cross-sectional areas as input data to the "working" model.

Validation is a necessary but not sufficient condition for "working" model acceptance. Subtle "bugs" in the program, program logic, or the numerical solution itself may occur well into the application of the model when unforeseen cases are run. No amount of validation testing is enough, and usually a wise choice of several validations is made, depending on the particular type of "working" model. The final result of validation is a functional model, i.e., a tested, "working" model.

PHILOSOPHY UNDERLYING PARAMETER ESTIMATION FOR WATER QUALITY MODELS

by

Carl W. Chen[1]
Steven A. Gherini[2]

Introduction

Water quality models possess several properties useful to decision makers. They predict the consequences of various engineering alternatives proposed for environmental improvement or for mitigation of deleterious effects. They also provide technical bases for explaining why and how environmental benefits are to be accrued by the proposed actions.

For decision makers to accept the conclusions based upon a quality model, the model must be credible. Credibility can be enhanced by using a model that is based upon sound scientific principles, that has had several previous successful applications for different prototypes, that is readily calibrated to the system being modeled, and that has been verified for the aquatic system in question using data sets independent of those used for calibration.

The purpose of parameter estimation is to improve model calibration and therefore credibility. Parameter values are selected that result in adequate comparisons between the observed and the predicted water quality data.

A discussion of parameter estimation cannot be provided without making reference to other related issues, e.g., model complexity, rates and expressions included, and the boundary conditions for the system being modeled. All these factors influence the number of parameter values to be estimated and the degree of empiricism involved.

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The ultimate test of a model rests in its ability to reproduce the observed data. Since the model, regradless of its complexity, is a simplified approximation of the prototype, it can never simulate exactly all perturbations experienced by the real system. Discrepancies invariably exist due to the errors introduced by idealization of the prototype and/or due to errors in the measurement of the field data. The problem of parameter estimation is this: How can parameter values for a model be selected and adjusted to minimize the errors in prediction.

Model Complexities

It is generally agreed that one should use the simplest possible model appropriate for the analyses. The term "simple", however, is relative, and is difficult to define. A model that is "simple" to some may be complex to others.

Simple models do have special appeal to decision makers looking for simple answers. They are attractive in that they are sometimes inexpensive to use both in terms of time and costs. They can be explained in a straightforward manner. These may be illusionary, however.

Many aquatic systems are too complex to be handled by simple models. Simple models often require unrealistic idealization of the prototype and negate many benefits of modeling, e.g., keeping track of all the complex interactions and feedback known to exist in the real system.

Nonetheless, it is up to the analyst to devise the simplest possible model that will answer the questions of interest. Sometimes the analyst must acknowledge the need for a reasonably detailed model. To be accepted, they must also learn how to explain the model simply regardless of its complexity, preferably in layman's language, so that it can be understood.

To help decision makers understand issues, it is important to discuss what water quality models are and how simple water quality models are derived. Water quality models usually operate on a grid system designed to provide spatial representation of the water body. Each grid point can accept input described by such boundary conditions as river inflows, waste inputs, river outflows, and climatology.

Mathematical equations with appropriate coefficients are formulated to describe the physical processes that transport materials from one grid point to others; the chemical transformations that take place within the water volume represented by the grid point; and biological processes such as nutrient uptake, growth, respiration, mortality, and grazing.

Up to this point the various physical and chemical characteristics of the prototype are considered in great detail. That is, the total physical system is divided into smaller units and the prototype behavior is dissected into a series of simultaneous reactions, represented by differential equations. An integration step must follow to produce answers.

The equations are solved by a computer to produce a time history of water quality at each grid point. The rates of various physical, chemical and biological transformations can be printed for a detailed analysis on the relative importance of various factors contributing to observed water quality (e.g., physical pollution transport, chemical interactions, and organism growth).

Model simplification is accomplished by aggregating the grid points, by taking a larger time step of computation, and/or by excluding certain formulations (and therefore processes) from the model. As the model is simplified, however, more empiricism and more external parameter estimation is required. For example, if the model does not include hydrodynamic calculations, the flow field must be estimated. When zooplankton, for example, are excluded from the calculations, one must provide an estimate of the phytoplankton loss to account for grazing by zooplankton.

Developing estimates for the added parameters is not easy. They are intrinsic system properties that can not be estimated _a priori_. Their values in fact adjust themselves to the environmental stimuli and therefore are not constants. To provide good estimates for those parameter values, one needs extensive field data. The current data required to support a simplified model can be several orders of magnitude more extensive than those required for occasional checks against the output of hydrodynamic calculations.

Further, the simplified models may calculate so-called "average concentrations" for large areas over a relatively long time. Such "average concentrations" cannot be compared directly to observed data. Field observations are made at discrete points in time. The observed data must be averaged before they can be compared to the model output. How this "averaging" should be done is not always apparent.

The point being made here is that oversimplification of a model can be as bad as overcomplication. It is not axiomatic that a simple model requires simple data and hence simple parameter estimates.

Nondesignated 208 Approach

Under the sponsorship of the Environmental Research Laboratory (Athens, Georgia), Tetra Tech has developed a three-part program for water quality analysis in nondesignated 208 areas in the United States.

The first part is screening where very simple models are used. The calculations are such that they can be performed with desktop calculators. A manual has been prepared detailing the methodology, data needs, calculation procedures and limitations. The manual has four sections describing the methods for analyzing wasteloads (point and nonpoint sources), and for predicting pollutant distributions in rivers, lakes, and estuaries.

The purpose of the screening methodology is to help identify problem areas for more detailed analyses. While the methodology is an estimation tool, and is not rigorous from a modeling standpoint, it can serve as an educational tool for the non-modeler. An appreciation of the basic principles underlying more complex models can be gained by examining the procedures.

For the problem areas identified, a more sophisticated analysis may be called for. The second part of the program is a series of mathematical models that can be used for that purpose.

The third part of the program is the "rates manual", which serves as a companion to the first two parts. In this manual, the rates, constants, and kinetics formulations used in surface water quality modeling have been compiled and analyzed. The definition of each parameter, how it is used in the model, and ranges of parameter values reported in the literature are presented. The subject areas include various physical, chemical, and biological processes. Detailed information is provided for reaeration, dissolved oxygen saturation, photosynthesis, carbonaceous deoxygenation, nitrogenous deoxygenation, benthic oxygen demand, coliform bacteria die-off, algal and zooplankton dynamics.

Calibration Procedure

While there are autocalibration programs available, they must be used with care. The manual procedure of adjusting coefficients for best fit is favored, because one can learn a great deal about the system behavior by trying to resolve differences between model predictions and observed data. By leaving calibration to the computer, the model may well be calibrated improperly.

For manual calibration, it is important for investigators to select parameter values within the ranges reported in the literature. In that respect, the "rates manual" described previously will be useful.

In comparing calculated and observed water quality data, one should use several approaches. The temporal variations at selected locations and the spatial variations at selected times may be compared for the overall fit. After that, the point differences between the observed and the calculated values can be determined for a statistical evaluation of precision.

Model output can be shown to have varying sensitivity to different classes of parameters. Parameter classes, ranked in typical order of decreasing influence on model output, are presented below:

- Boundary conditions
- Coefficients for physical processes
- Coefficients for chemical processes, and
- Coefficients for biological processes

To improve calibration, one should adjust first the most sensitive coefficient (i.e., boundary conditions) followed by the less sensitive parameters. The procedure is to change the most sensitive parameter in one direction (e.g., from a large to a small value) until further improvement on the calibration cannot be made and then do the same for the next most sensitive parameter.

Error Analysis

It is important to understand that there will always be discrepancies between the observed and the predicted water quality. Errors are most commonly introduced by the following factors:

- The boundary conditions are more variable in the prototype than those assumed for the model.

- Prototype processes are more complex than the simplified formulations used.

- Rate coefficients have random variations not accounted for in the model.

- There are errors in the field measurements.

All model studies should include sensitivity analysis to quantify the relative magnitude of error associated with each of the above factor groups.

New Field Programs

Many historical data sets available for water quality modeling studies are incomplete. Most data sets contain the water quality measurements within the aquatic system without simultaneous measurement of boundary conditions, i.e., hydrologic inputs, pollution loads and meteorology.

Modelers are often hard-pressed to come up with the estimates needed for their modeling work. Given inadequate data, constant boundary conditions are often assumed and imposed on the model. Nonetheless, the model is still expected to perform the impossible task of simulating variable water quality conditions observed in the field.

Recently, we have been involved in a very exciting program where modeling studies and field research activities are being performed concurrently and in a coordinated manner. The purpose of the program is to gain understanding of the processes involved in the neutralization of acidic precipitation. As a focal point the following task has been delineated: Determine why three lakes in the Adirondack Mountains of New York exhibit differing water quality (pH, alkalinity, etc.) in response to seemingly similar inputs of acid rain. One lake has a pH of about 7, one is acidic with a pH of 4-5, and one has a variable pH ranging from 4 to 7. What must be discovered is how various physical, chemical and biological processes within the basin interact to produce these effects.

The program is being sponsored by the Electric Power Research Institute (Palo Alto, California). Six universities and one private company are working together to research important processes in and to measure various state variables throughout the system which includes atmospheric, terrestrial, and aquatic components. Two national laboratories and two other federal agencies are also participating in the field research program. Field measurements are synchronized so that basin input, basin output, and system state variables are monitored simultaneously.

The field program has been designed based in part upon a conceptual model formulated to follow the quantity and quality of precipitation (rain or snow) from the tree top, through the canopy, soil horizons, bogs, stream reaches and lakes. The model was conceptualized based on an extensive review of literature.

The hydrologic section of the model has already been developed. At the preliminary calibration stage, the model has been used to bracket the depths of flow in the saturated zone of soils, the likely permeabilities of the soil horizons and other geohydrological characteristics. This information is used to help refine the field sampling program design.

The field program has been underway for 18 months and will continue for another two and one-half years. The first two years' data will be used to calibrate the model; the last two years' data will be used for verification. Based on the results obtained to date, there are reasons to believe that this coordinated modeling/field research program will prove successful.

It is true that not many studies can be conducted in such depth. On the other hand, Federal monies have too often been spread so thinly on so many projects that very little return per dollar spent has been witnessed. Decision makers often fail to get the facts upon which to base their decisions, and modelers continue to be blamed for not having been able to properly test and calibrate their models. If modelers are expected to contribute, they must be supported to do what is right, not simply what is inexpensive.

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MEASURES OF VERIFICATION

by

Robert V. Thomann[1]

Introduction

There are two basic reasons for constructing representations of natural water systems through mathematical modeling. First is the need to increase the level of understanding of the cause-effect relationships operative in water quality and secondly, to apply that increased understanding to aid the decision making process. Water quality models are largely syntheses of a number of phenomena; water transport, complicated reaction kinetics, and externally generated residuals inputs. The builder of water quality models acts as one part of a three part interaction which includes the specialist who generates process details (e.g., uptake of nutrients by phytoplankton) and the manager who is concerned with the problem specification and ultimately its resolution in some sense. Figure 1 shows this interaction.

For more than fifty years now, this relationship has continued in a great variety of increasingly complex water quality modeling situations. But one of the common threads throughout this period has been the constantly recurring question of the validity, credibility, and utility of the water quality models. Indeed even in the historical roots of water quality modeling, as embodied in the famous Ohio River dissolved oxygen studies of the 1920's, this question of model validity was present. Resurveys of the Ohio River between 1914 and 1930 were considered critical to a justification of the basic history theory of deoxygenation and reaeration (Crohurst, 1933). Indeed the works of Streeter and Phelps (1925) addressed the question of model validity quite directly by numerous qualitative comparisons to observed data and through quantitative comparisons by computing, for example the root mean square error between dissolved oxygen theoretical calculations and observed values. One easily gains the impression from a reading of these early works that analysis of the relationships between observed and computed values, both qualitatively and statistically was a normally acceptable and expected procedure

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As the issues of water quality become more complex, requiring the interaction of numerous variables in space and time, the questions of model credibility increase. The responses to these questions often tend to be somewhat qualitative; e.g., "The results appear reasonable" or "The major features of the observed behavior have been captured" or "The comparison between observed and computed values is marginal but sufficient for most purposes." Increasingly, most assessments of model validity do not seem to directly answer the basic questions of the manager, the specialist or the general public. Common questions are: "How good is the model?", "What is the level of confidence that we can place on your results?", "How do two models purporting to represent the same water quality phenomena compare to each other?"

In the light of the questions raised on model credibility, it is appropriate to address the issue of what measures of verification, if any, might be useful in today's water quality modeling setting. However, a brief review of the principal components of a water quality model is necessary to clarify and propose some language that might be applicable to this issue of model verification. Within the context of water quality problems, the basic issues discussed apply also to models of input generation and water transport.

Figure 2 shows the principal components of a mathematical modeling framework. The upper two steps enclosed with the dashed lines, namely "Theoretical Construct" and "Numerical Specification" constitute what is considered a mathematical model. This is to distinguish the simple writing of equations for a model from the equally difficult task of assigning a set of representative numbers to inputs and parameters. Following this initial model specification are the steps of a) model calibration, i.e., the first "tuning" of model output to observed data and b) the step of model verification i.e., the use of the calibrated model on a different set of water quality data. This verification data set should presumably represent a condition under a sufficiently perturbed condition (i.e., high flows, decreased temperature, changed waste input) to provide an adequate test for the model. Upon the completion of this verification or auditing step, the model would be considered verified.

Stages of Model Credibility

The following definitions are therefore offered:

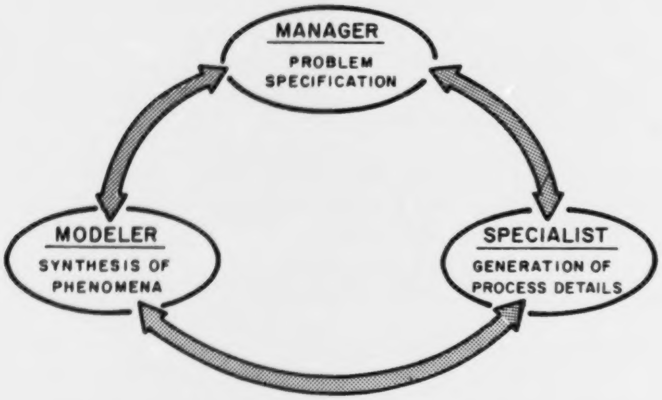

MANAGER
PROBLEM SPECIFICATION
MODELER
SYNTHESIS OF PHENOMENA
SPECIALIST
GENERATION OF PROCESS DETAILS

FIGURE I. RELATIONSHIP BETWEEN MODELER, SPECIALIST AND MANAGER IN WATER QUALITY

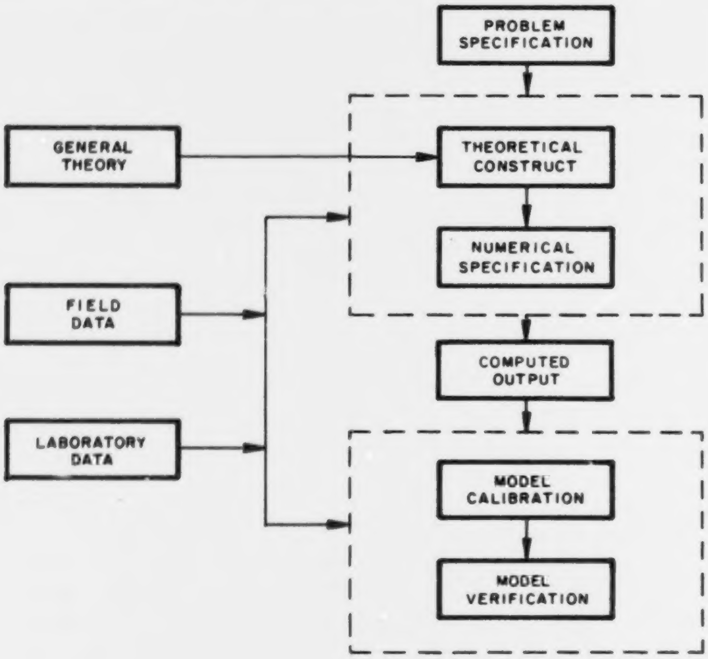

PROBLEM SPECIFICATION
GENERAL THEORY
THEORETICAL CONSTRUCT
NUMERICAL SPECIFICATION
FIELD DATA
COMPUTED OUTPUT
LABORATORY DATA
MODEL CALIBRATION
MODEL VERIFICATION

FIGURE 2. PRINCIPAL COMPONENTS OF MATHEMATICAL MODELING FRAMEWORK

1. Model: A theoretical construct, together with assignment of numerical values to model parameters, incorporating some prior observations drawn from field and laboratory data, and relating external inputs or forcing functions to system variable responses.

2. Model Calibration: The first stage testing or tuning of a model to a set of field data, preferably a set of field data not used in the original model construction; such tuning to include a consistent and rational set of theoretically defensible parameters and inputs.

3. Model Verification: Subsequent testing of a calibrated model to additional field data preferably under different external conditions to further examine model validity.

The calibrated model, it should be noted, is not simply a curve-fitting exercise, but should reflect wherever possible more fundamental theoretical constructs and parameters. Thus, models that have widely varying coefficients (i.e., deoxygenation coefficients) to merely "fit" the observed data are not considered calibrated models.

The verified model is then often used for forecasts of expected water quality under a variety of potential scenarios. However, it is apparently rare that following a forecast, and a subsequent implementation of an environmental control program, that an analysis is made of the actual ability of the model to predict water quality responses. This can be termed a "post-audit" of the model, as shown in Figure 3. Somehow it seems that once a facility has been constructed, the federal and state agencies, municipalities, and industries are somewhat reluctant to return to the scene of a water quality problem to monitor the response of the water body. A fourth step therefore in determining model credibility is suggested as follows:

4. Model Post-Audit: A subsequent examination and verification of model predictive performance following implementation of an environmental control program.

Need for Measures of Verification

Increase in Model Complexity. The most obvious need for some measures of model verification is the fact that water quality models have increased greatly in complexity. Figures 4-7 illustrate this progression. From relatively simple two linear system models of biochemical oxygen demand and dissolved oxygen for the first forty years of model development to the new complex non-linear interactive eutrophication and toxic substances models, the ability to describe model performance has become increasingly difficult. The number of state variables in some models has increased dramatically. It is not unusual today

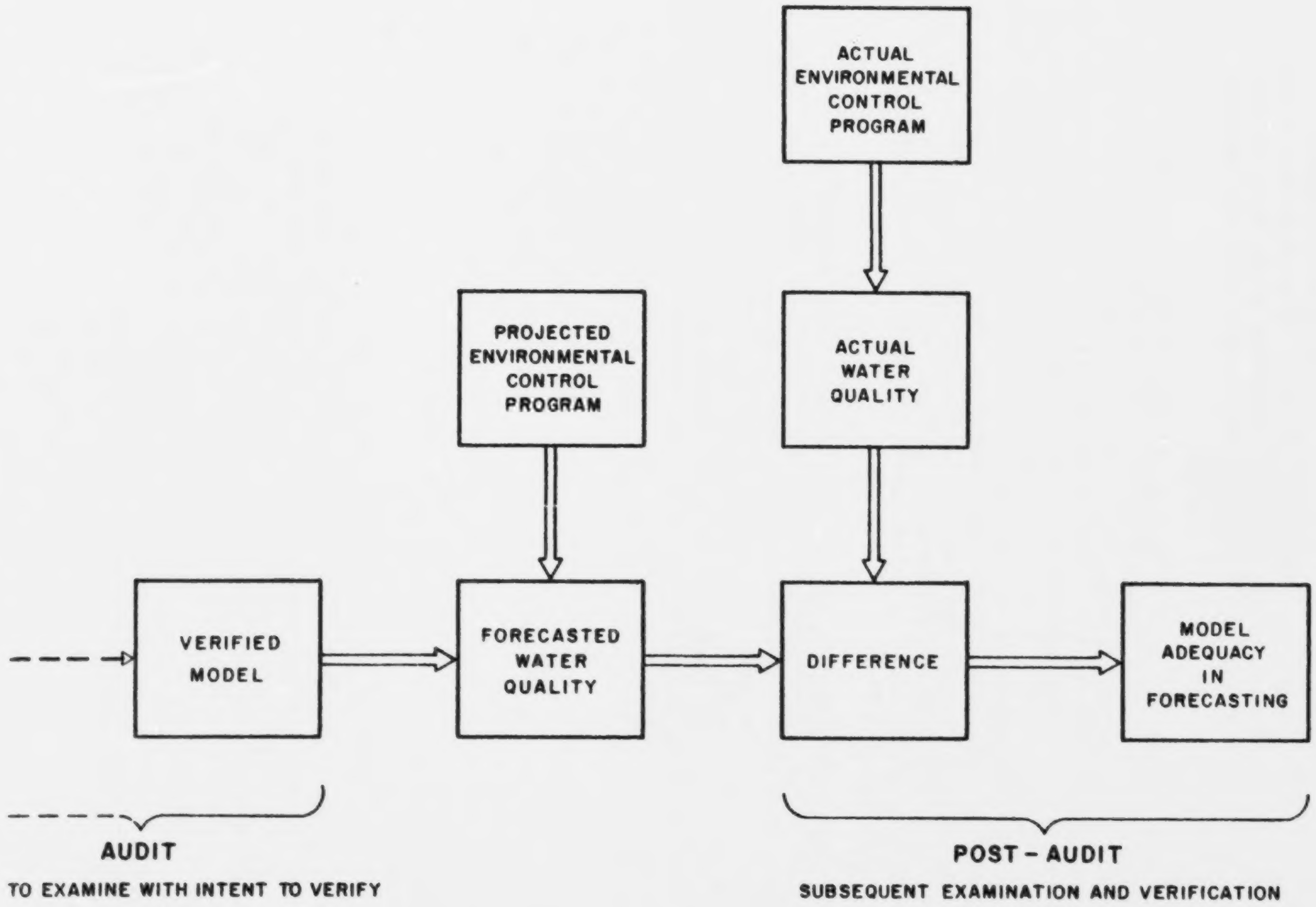

ACTUAL ENVIRONMENTAL CONTROL PROGRAM
PROJECTED ENVIRONMENTAL CONTROL PROGRAM
ACTUAL WATER QUALITY
VERIFIED MODEL
FORECASTED WATER QUALITY
DIFFERENCE
MODEL ADEQUACY IN FORECASTING
AUDIT
TO EXAMINE WITH INTENT TO VERIFY
POST - AUDIT
SUBSEQUENT EXAMINATION AND VERIFICATION

FIGURE 3. AUDITING AND POST AUDITING OF WATER QUALITY MODELS

to construct models with up to 20 or more state variables. Furthermore, as illustrated in Figures 4-7, the physical dimensionality now encompasses the range from the more traditional one-dimensional streams to fully three-dimensional estuaries, bays and lakes.

As the number of state variables and physical dimensionality has increased, the overall ability of the analyst to comprehend model output has decreased. This is simply due to the overall size of the model. For example, if a "compartment" is considered as a state variable, i = 1,...m, positioned at some spatial location j = 1...n, then the total number of compartments to be solved for a fully interactive model is m times n. Figure 8 shows the growth of the number of model compartments since the earliest work of the two state variable problems of BOD and DO. The almost explosive growth in the number of model compartments, coincidental with passage of major water quality legislation is evident.

Increase in Complexity of Questions. The second major reason for some quantitative measures of verification is the fact that the level of questions in water quality has increased in complexity. Many of the water quality issues today extend well beyond the traditional problem of raw or inadequately treated sewage. In that traditional framework, it generally was clear that some treatment of municipal sewage would probably improve water quality, specifically dissolved oxygen. However, some of the water quality questions today may involve such complex interactions that it is not clear that certain environmental controls will in fact produce the classical result. The Potomac estuary eutrophication problem is a case in point. It is not clear that nitrogen removal at the Washington, D.C. Blue Plains plant actually will result in any reduction in the phytoplankton population that could not be achieved solely by phosphorus control. Similarly, it is not entirely clear that extensive dredging of PCB deposits in the Upper Hudson will result in a reduction of the PCB body burden of the striped bass in the Lower Hudson estuary to levels below the FDA requirement.

The complexity of the problem then leads to the very real possibility that environmental control measures may be called for by model predictive analyses when in fact the implementation of such controls may produce little or no response in water quality. The economic, political, and social consequences of "wrong" answers therefore become more acute in today's problem setting. Some quantifiable measure of model performance in improving understanding or predictive performance would seem, therefore, to be of considerable importance.

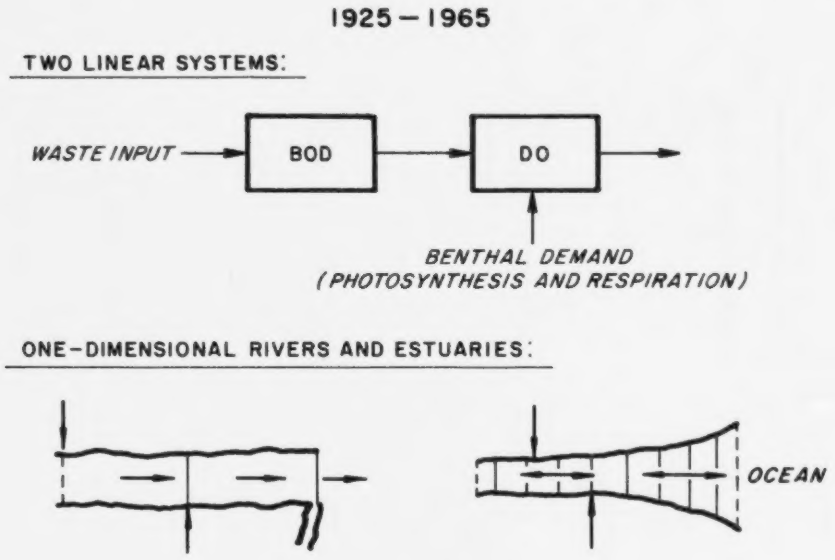

1925 — 1965
TWO LINEAR SYSTEMS:
WASTE INPUT
BOD
DO
BENTHAL DEMAND
(PHOTOSYNTHESIS AND RESPIRATION)
ONE-DIMENSIONAL RIVERS AND ESTUARIES:
OCEAN

FIGURE 4. WATER QUALITY MODELS, 1925-1965

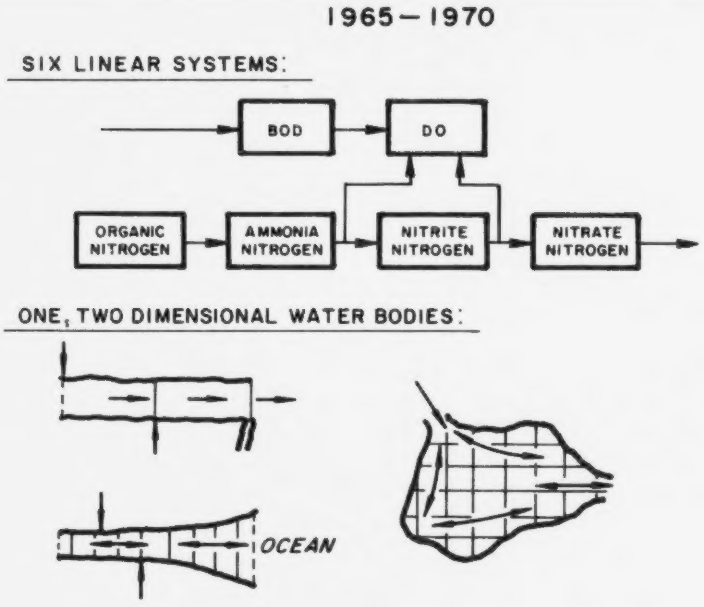

1965 — 1970
SIX LINEAR SYSTEMS:
BOD
DO
ORGANIC NITROGEN
AMMONIA NITROGEN
NITRITE NITROGEN
NITRATE NITROGEN
ONE, TWO DIMENSIONAL WATER BODIES:
OCEAN

FIGURE 5. WATER QUALITY MODELS, 1965-1970

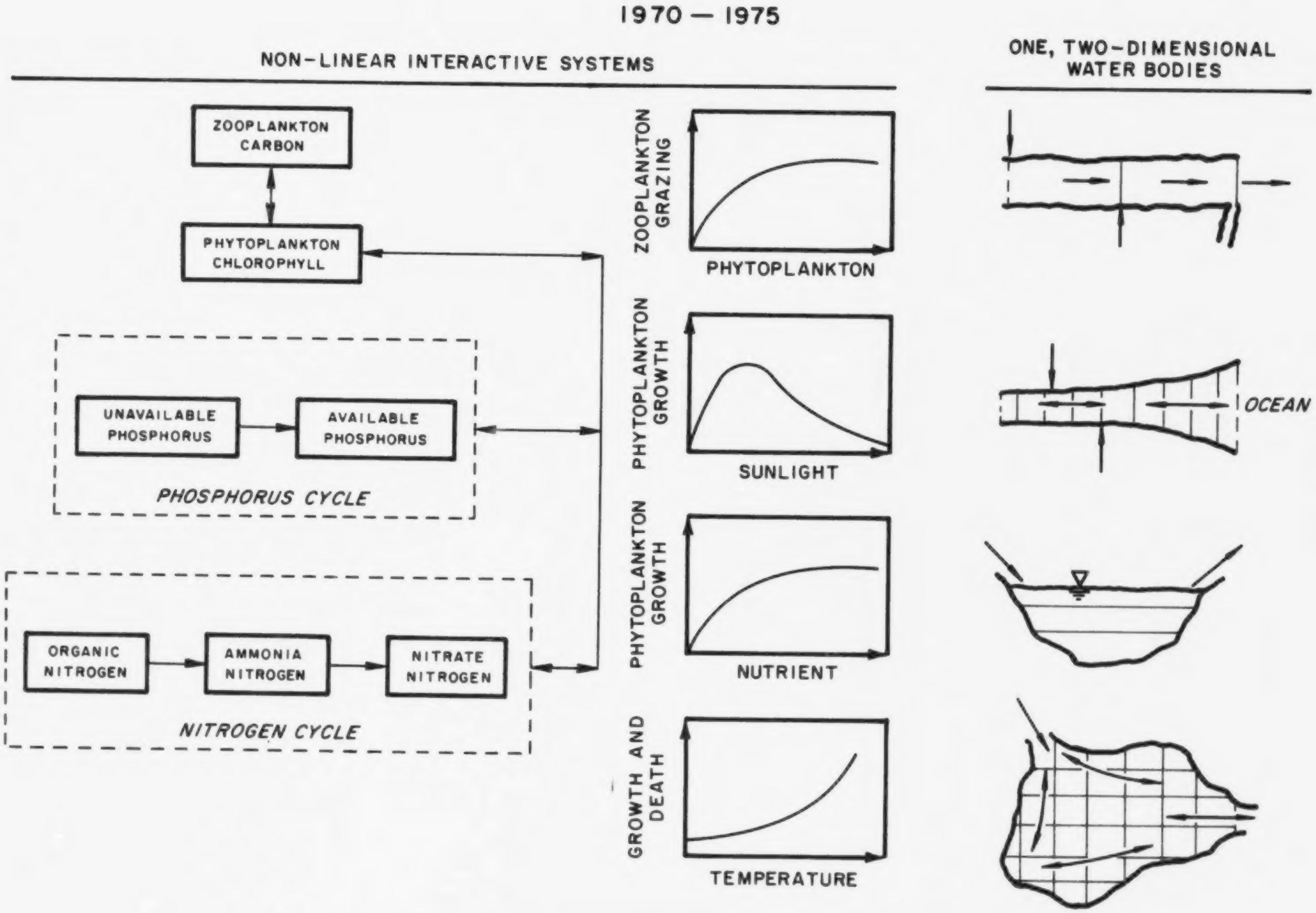
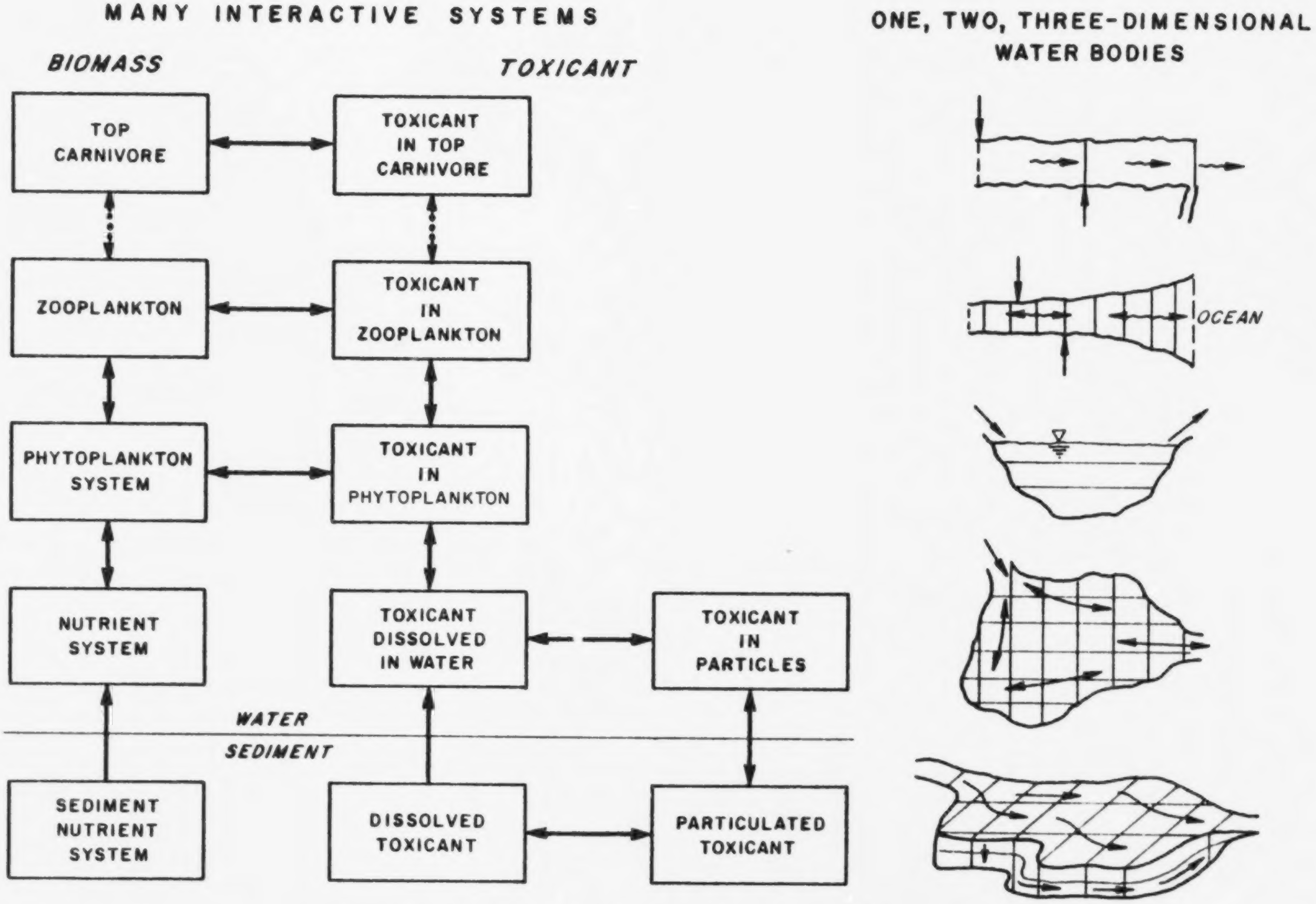

1970 — 1975
NON-LINEAR INTERACTIVE SYSTEMS
ONE, TWO-DIMENSIONAL WATER BODIES
ZOOPLANKTON CARBON
PHYTOPLANKTON CHLOROPHYLL
UNAVAILABLE PHOSPHORUS
AVAILABLE PHOSPHORUS
PHOSPHORUS CYCLE
ORGANIC NITROGEN
AMMONIA NITROGEN
NITRATE NITROGEN
NITROGEN CYCLE
ZOOPLANKTON GRAZING
PHYTOPLANKTON
PHYTOPLANKTON GROWTH
SUNLIGHT
PHYTOPLANKTON GROWTH
NUTRIENT
GROWTH AND DEATH
TEMPERATURE
OCEAN

FIGURE 6. WATER QUALITY MODELS 1970-1975



MANY INTERACTIVE SYSTEMS

ONE, TWO, THREE-DIMENSIONAL WATER BODIES

BIOMASS
TOXICANT
TOP CARNIVORE
TOXICANT IN TOP CARNIVORE
ZOOPLANKTON
TOXICANT IN ZOOPLANKTON
PHYTOPLANKTON SYSTEM
TOXICANT IN PHYTOPLANKTON
NUTRIENT SYSTEM
TOXICANT DISSOLVED IN WATER
TOXICANT IN PARTICLES
WATER
SEDIMENT
SEDIMENT NUTRIENT SYSTEM
DISSOLVED TOXICANT
PARTICULATED TOXICANT
OCEAN

FIGURE 7. WATER QUALITY MODELS 1975-?

Some Verification Measures

Qualitative Measures

Probably the most direct and easily understood measure of model performance is to present qualitative comparisons of observed data and computed values. This is most often done in the form of overplotting data and theory or tabulating the comparison between the two and then drawing qualitative judgmental conclusions about the adequacy of the model and its suitability for projection purposes. A plot of data versus theory can be a most graphical measure of model credibility - easily understood and clearly visual. But for some problems, such a simple qualitative measure is not possible or simply not adequate. This is particularly so for time variable models of several state variables and multi-dimensional systems. For models of this type, as well as the simpler model framework, some statistical comparisons may provide further understanding of model credibility.

Statistical Comparisons

A variety of simple statistical comparisons may be appropriate to quantify model verification status. Such measures would be intended to supplement the qualitative comparisons. Examples of statistical analyses between observed and computed values are:

1) Regression analyses
2) Relative error
3) Comparison of means
4) Root mean square error

1) Regression Analyses

A perspective on the adequacy of a model can be obtained by regressing the calculated values with the observed values. Therefore, let the testing equation be

$$\bar{x} = \alpha + \beta\bar{c} + \varepsilon \qquad (1)$$

where α and β are the true intercept and slope respectively between the calculated values, $\bar{c}$, and the observed values, $\bar{x}$, and ε is the error of $\bar{x}$. The regression model equation (1) assumes, of course, that $\bar{c}$, the calculated value from the water quality model, is known with certainty which is not the actual case. With equation (1), standard linear regression statistics can be computed, including

a) The square of the correlation coefficient, r^2, (the % variance accounted for) between calculated and observed

b) Standard error of estimate, representing the residual error between model and data

c) Slope estimate, b, of β and intercept estimate, a, of α

d) Test of significance on the slope and intercept. The null hypothesis on the slope and intercept is given by $\beta = 1$ and $\alpha = 0$. Therefore, the test statistics

$$\frac{b-1}{s_b} \text{ and } \alpha/s_a$$

are distributed as student's t and n-2 degrees of freedom. The variance of the slope and intercept, s_b^2 and s_a^2 are computed according to standard formulae. A two-tailed "t" test is conducted on b and a, separately, with a 5% probability in each tail, i.e. a critical value of t of about 2 provides the rejection limit of the null hypothesis.

Regressing the calculated and observed values can result in several situations. Figures 9(b) and (c) shows that very good correlation may be obtained but a constant fractional bias may exist ($b<1$, $b>1$); also Figure 9(a) indicates that poor correlation may be obtained with slope = 1 and intercept = 0. Finally, Figure 9(d) indicates the case of good correlation but for an $a > 0$ a constant bias may exist. Evaluation of r^2, b and a, together with the residual standard error of estimate, can provide an additional level of insight into the comparison between model and data.

2) Relative Error

Another simple statistical comparison is given by the relative error defined as

$$e = \frac{|\bar{x} - \bar{c}|}{\bar{x}} \tag{2}$$

Various aggregations of this error across regions of the water body or over time can also be calculated and the cumulative frequency of error over space or time can be computed. Estimates can then be made of the median relative error as well as the 10% and 90% exeedance frequency of error. The difficulties with this statistic are its relatively poor behavior at low values of $\bar{x}$ and the fact that it does not recognize the variability in the data. In addition, the statistic is poor when $\bar{x} > \bar{c}$ since under that condition the maximum relative error is 100%. As a result, the distribution of this error statistic is most poorly behaved at the upper tail. Nevertheless, if the median error is considered, this statistic is a readily understood comparison and provides a gross measure of model adequacy. It can also be especially useful in comparisons between models.

3) Comparison of Means

A third measure is to conduct a simple test of the differences between the observed mean and the computed mean. Letting $\bar{d} = \bar{x} - \bar{c}$, the test statistic distributed as a student's "t" probability density function is given by

$$t = \frac{\bar{d} - \delta}{s_{\bar{d}}} \tag{3}$$

where δ is the true difference between model and data and $s_{\bar{d}}$ is the standard deviation of the difference given by a pooled variance of observed and model variability. If these latter quantities are assumed equal then

$$s_{\bar{d}} = \sqrt{2}s_{\bar{x}} \tag{4}$$

where $s_{\bar{x}}$ is the standard error of estimate of the observed data and is given by

$$s_{\bar{x}}^2 = \frac{s_x^2}{N} \tag{5}$$

4) Root Mean Square Error

Finally, a measure of the error between the model and the observed data is also given by the root mean square (rms) error as

$$r = \sqrt{\frac{\Sigma(x_i - c_i)^2}{N}} \tag{6}$$

As before, the rms error can be computed across a spatial profile or over time at a single location. The rms error is statistically well-behaved and provides a direct measure of model error. If expressed as a ratio to mean value (across a profile or over time), it represents a second type of relative error. The disadvantage of the rms error is that it does not readily lend itself to pooling across variables to assess overall model credibility.

Each of the above measures displays model credibility from different statistical viewpoints. Some are apparently useful

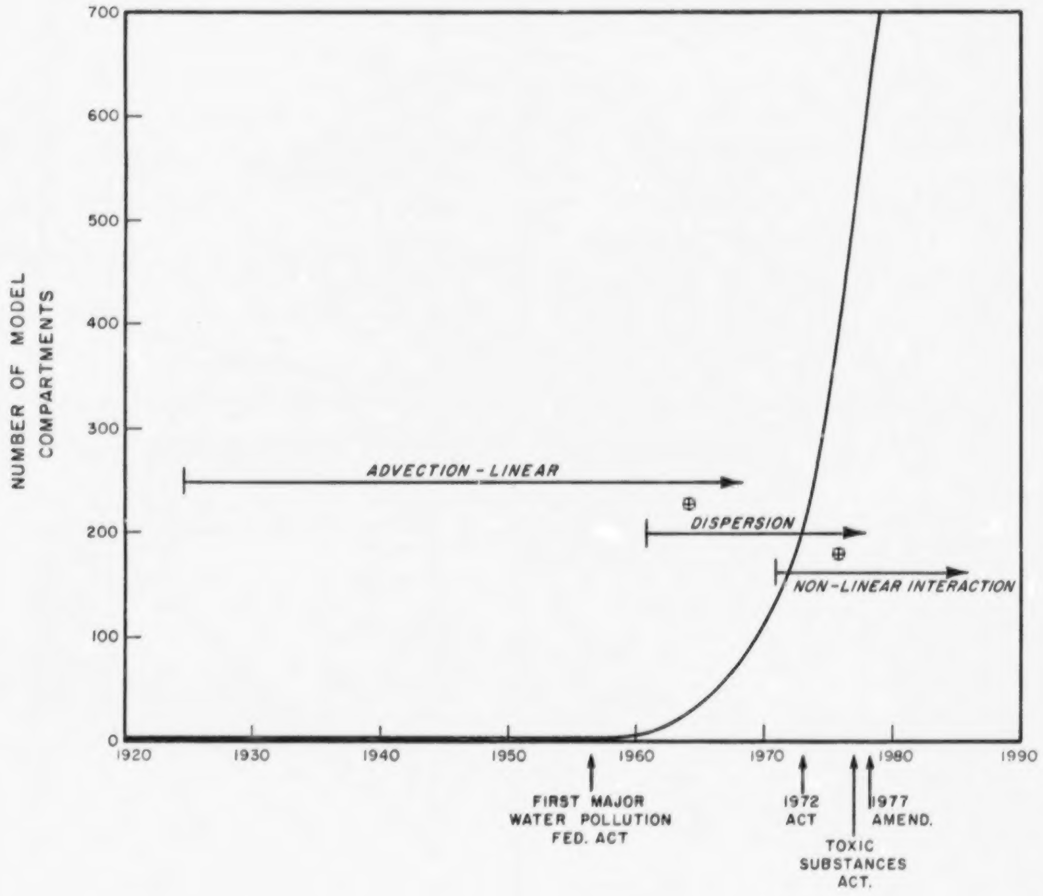


FIGURE 8. INCREASE OF NUMBERS OF MODEL COMPARTMENTS WITH TIME

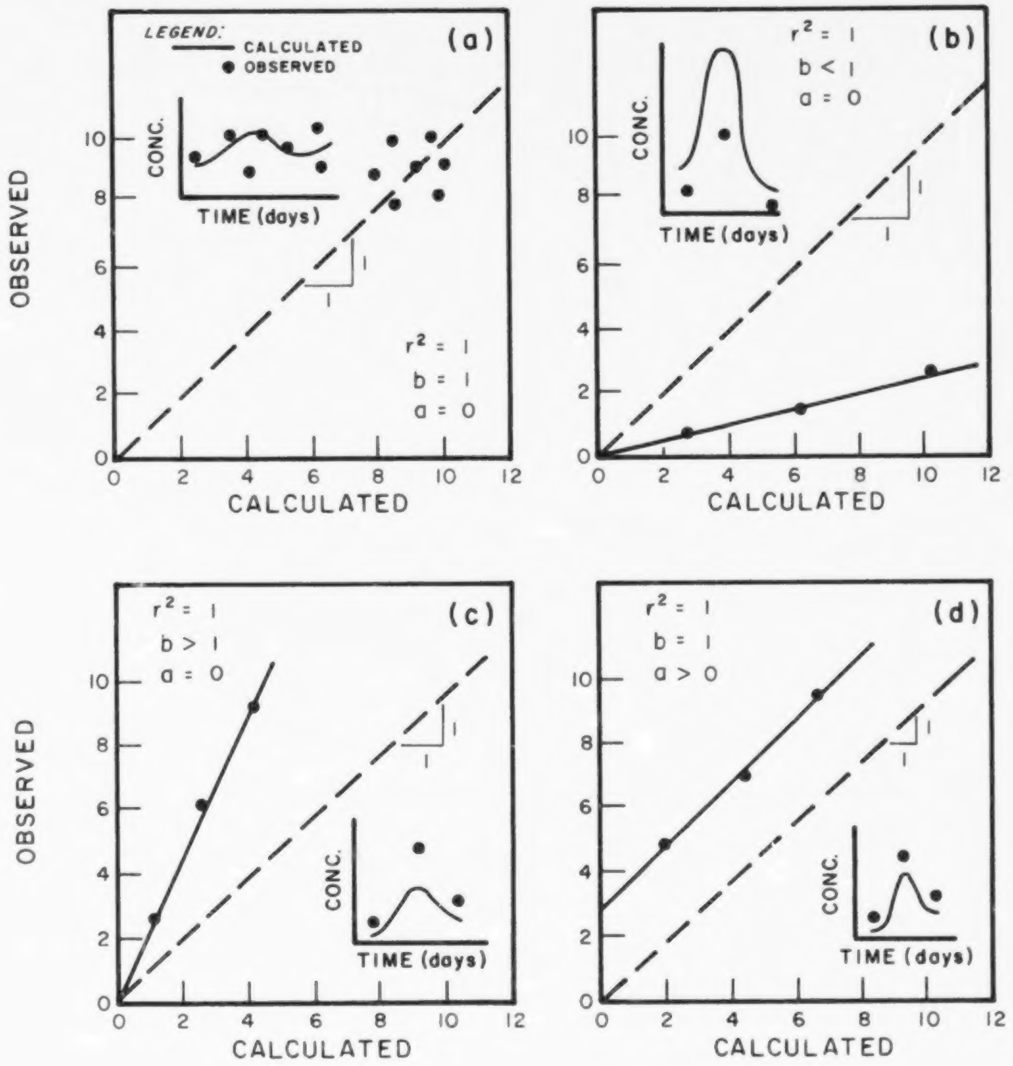


FIGURE 9. POSSIBLE CASES IN REGRESSION BETWEEN CALCULATED AND OBSERVED VALUES

for diagnostic purposes while others appear to be directly of value in succinctly describing model verification status.

Some Examples of Quantitative Verification Analyses

Dissolved Oxygen Models

In order to illustrate the present state of the art of model calibration/verification, a brief review was made of nineteen models of dissolved oxygen. This water quality variable was chosen since DO models have been the most extensively used and over the longest time period. The engineering reports for the fifteen water bodies were examined and relative errors, rms errors, and regression analyses were evaluated. All of the water bodies were analyzed by Hydroscience, Inc. It was assumed that the personnel engaged in the modeling analyses carried out the calibration/verification steps consistent with the definitions given above and not just to "curve fit" the model to the data.

The models included several small streams in New Jersey (less than 10 cfs), larger river systems such as the Ohio River and the Upper Mississippi River, bays and estuaries and a large model of the entire New York Harbor complex. A listing is shown in Table 1.

The distribution of the median relative error for these models is shown in Figure 10. For each water body, the error represents the median relative error where 50% of the stations (or times) had errors less than the values shown. Across all models, one-half of the models had median relative errors greater than 10% and one half of the models had median relative errors less than 10%.

As a crude measure, therefore, of the present state of the art of DO models calibration/verification, one might suggest an overall median relative error of 10%. It should, of course, be noted that this is not the error of actual prediction but merely the error representative of a present level of understanding of observed behavior of dissolved oxygen. The degree to which the results shown in Figure 10 is representative of all DO models is not known. More detailed analyses of a larger sample would be necessary.

Lake Ontario Eutrophication Models

A variety of models have been constructed of the eutrophication of Lake Ontario at several time and space scales and with different levels of kinetic detail (Thomann, et. al., 1979 and Thomann and Segna, 1979). Extensive application of the above quantitative measures of calibration/verification was made for a three-dimensional model of the Lake for one year and for a two segment vertical model over a ten year period.

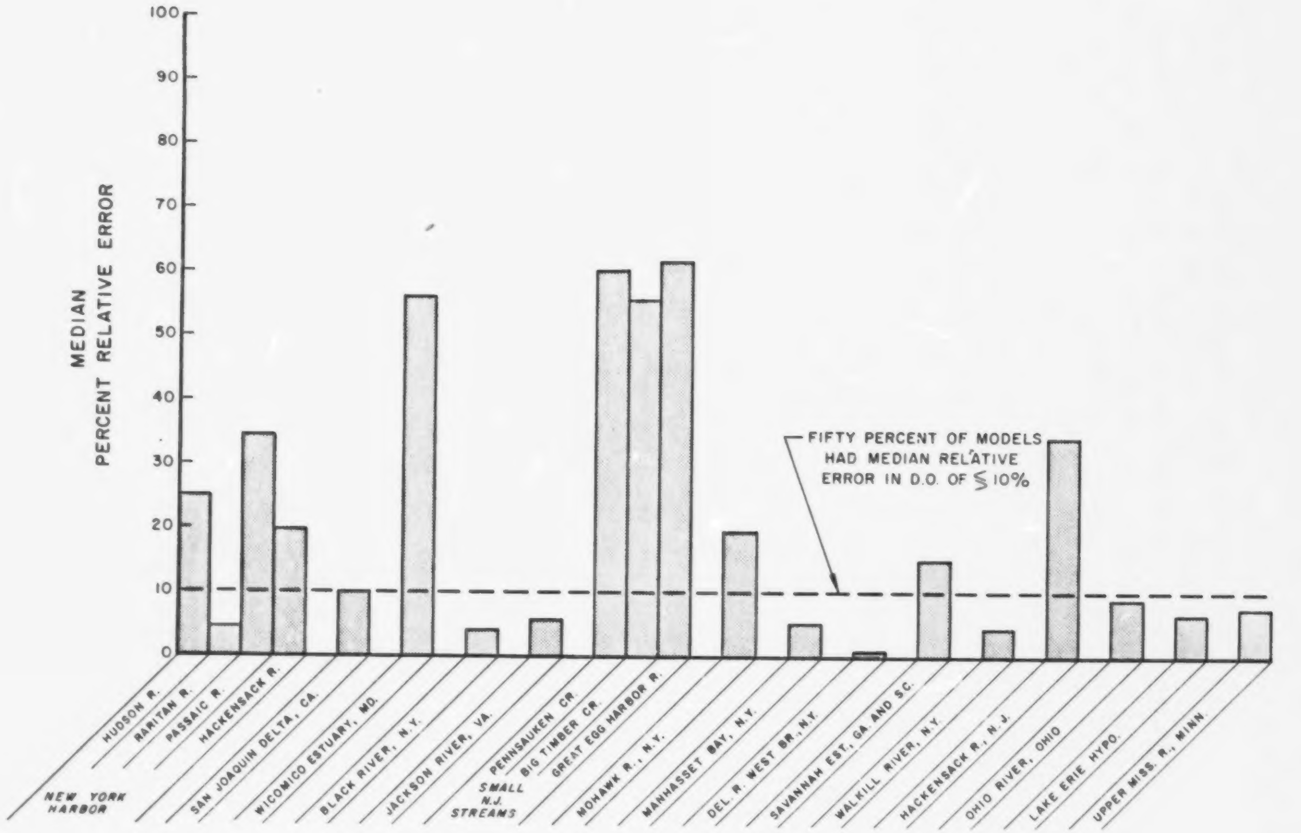


FIGURE 10. SOME RELATIVE ERRORS OF DISSOLVED OXYGEN MODELS

TABLE 1

WATER BODIES EXAMINED FOR DISSOLVED OXYGEN VERIFICATION STATISTICS

	Location	Remarks
1.	New York Harbor Hudson River Raritan River Passaic River Hackensack River	425 segment 3 Dimen. model
2.	San Joaquin Delta, Calif.	DO model part of eutrophication model
3.	Wicomico Estuary, Md.	A tidal tributary of Ches. Bay
4.	Black River, N.Y.	A tributary of Lake Ontario
5.	Jackson R., Va.	
6.	Small N.J. Streams 6a. Pennsauken Cr. 6b. Big Timber Cr. 6c. Grt. Egg Harbor R.	Tributaries of Delaware River and Bay
7.	Mohawk River, N.Y.	In vicinity of Utica, N.Y.
8.	Manhasset Bay, N.Y.	Bay of Long Island Sound
9.	Delaware R. West Br., N.Y.	
10.	Savannah Estuary, Ga., S.C.	
11.	Wallkill R., N.J.	
12.	Hackensack R., N.J.	
13.	Ohio R., Ohio	In vicinity of Cinn., Ohio
14.	Lake Erie Hypolimnion	DO model part of eutrophication model - time variable
15.	Upper Miss. R., Minn.	DO model part of eutrophication model - time variable

Figure 11 shows the median relative error across all variables at three levels of spatial aggregation - 67 segments, eight regions, and whole lake two layer scale. Five state variables were included in the pooled error (chlorophyll, total phosphorus, dissolved orthophosphorus, ammonia, and nitrate). The median relative error over the year was the highest at the smaller spatial scale (44%) and lowest at the whole lake scale (17%). This indicated that the model did not capture more local spatial phenomena as well as it reproduced overall lake behavior.

Figures 12-14 show the verification statistics from the analysis of 10 years of data on Lake Ontario using the two layer model. Two kinetic regimes are shown. Lake 1 kinetics are fairly standard and Lake 1-A kinetics included a more complex phytoplankton compartment (diatoms and non-diatoms), silica limitation and other kinetic changes in nutrient recycle. Figure 12 shows an example of the chlorophyll verification results for both regression analyses and relative error distribution. The regression results indicated some improvement in slope with the increased kinetic complexity but no improvement in the correlation or intercept. The median relative error for chlorophyll decreased from 42% to 30% with the inclusion of the more complex kinetics. Figure 13 shows the results of the student's t-test comparing observed and computed monthly means over the six state variables. For the indicated standard errors, the Lake 1-A kinetics gave a verification score of 70%, i.e., 70% of the variable-months where a comparison could be made showed no statistically significant difference between observed and computed means. If the standard errors are taken at one-half the values indicated, the score drops to 40%. Figure 14 shows the median relative errors for each variable and for all variables. The latter test indicated an overall relative error for the ten years of analysis and all variables of 22-32%.

A Suggestion

On the basis of the above concepts and illustrations together with the apparent growing need to be more definitive in assessing model credibility, it is suggested that quantitative measures of calibration and verification of models be an integral part of modeling whenever possible. This includes a pressing need to conduct post-auditing studies of model projections and resulting water quality.

The suggestion for quantitative measures of water quality model verification is aimed at responding to the many questions often raised at various stages in the decision making process. There are, however, advantages and disadvantages to quantitative measures of model verification. Some of the disadvantages are:

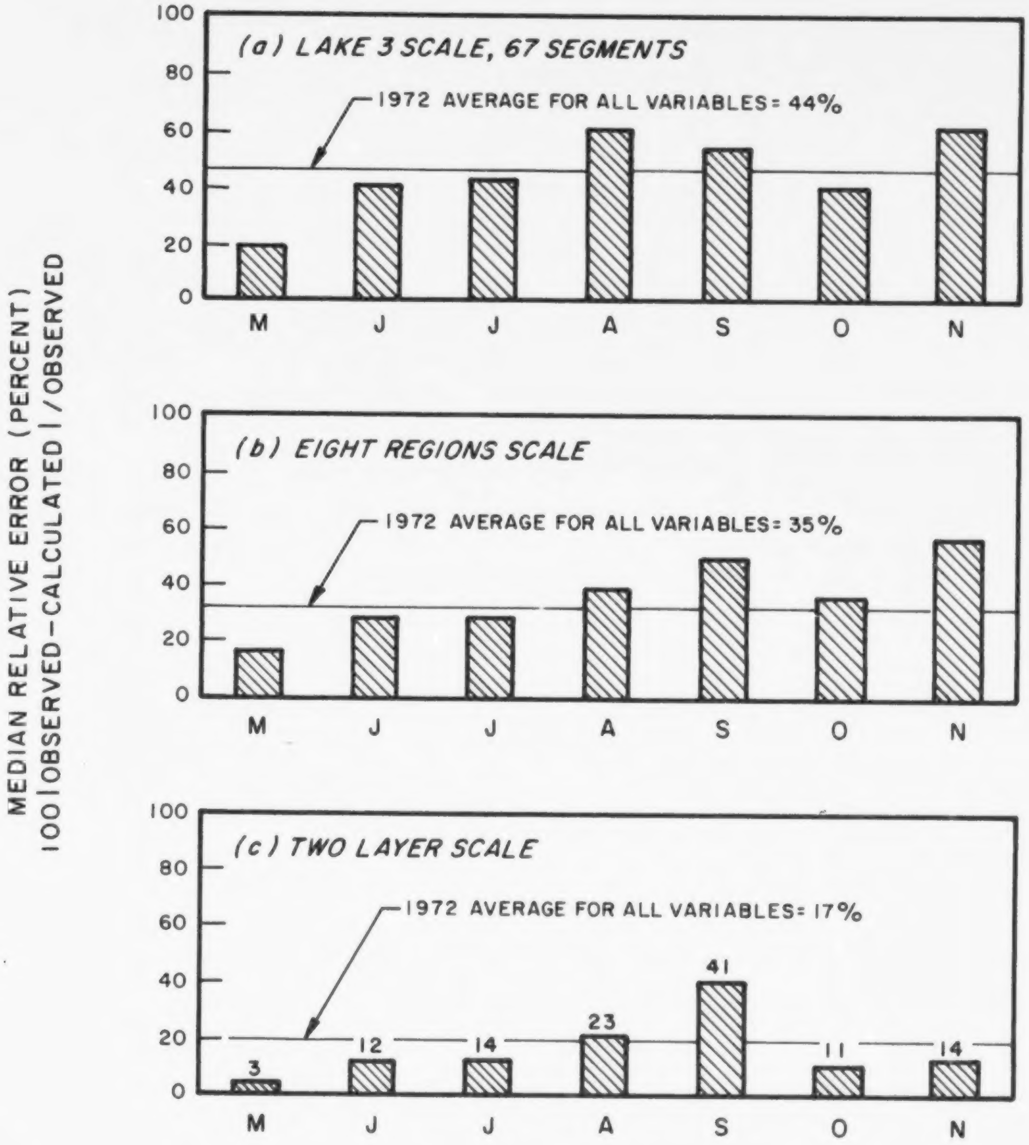


FIGURE 11. LAKE ONTARIO
MEDIAN RELATIVE ERROR AT THREE SPATIAL SCALES

THOMANN et al. 1979a

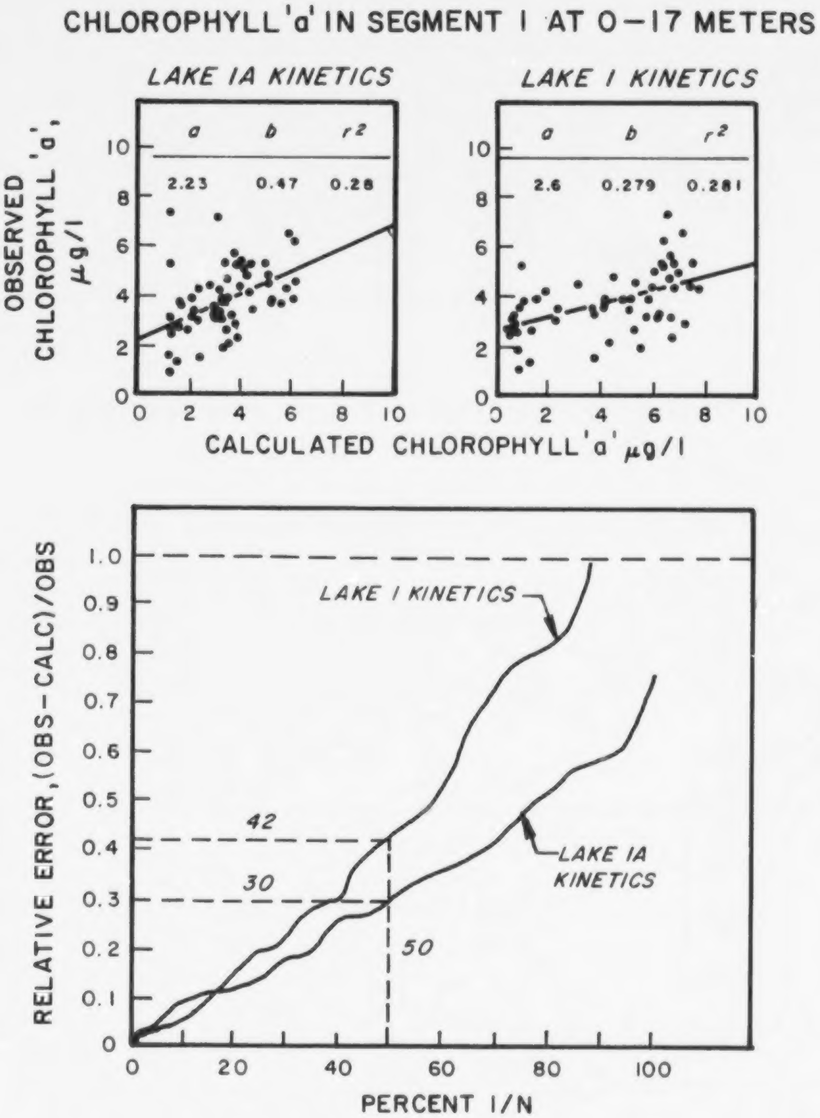


FIGURE 12. LAKE ONTARIO
CHLOROPHYLL VERIFICATION, TEN YEAR ANALYSIS

THOMANN AND SEGNA, 1979b

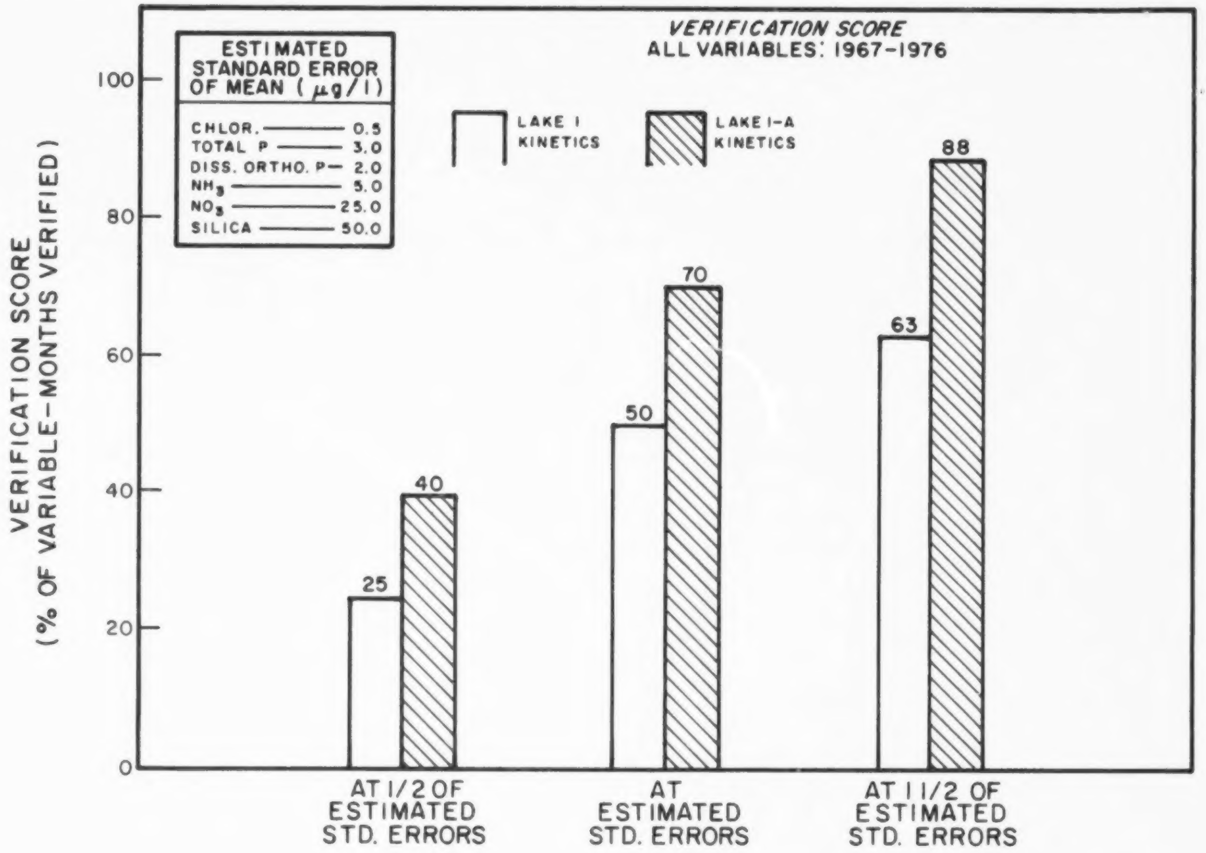


FIGURE 13. LAKE ONTARIO
VERIFICATION SCORES, ALL VARIABLES, TEN YEAR ANALYSIS

THOMANN AND SEGNA 1979b

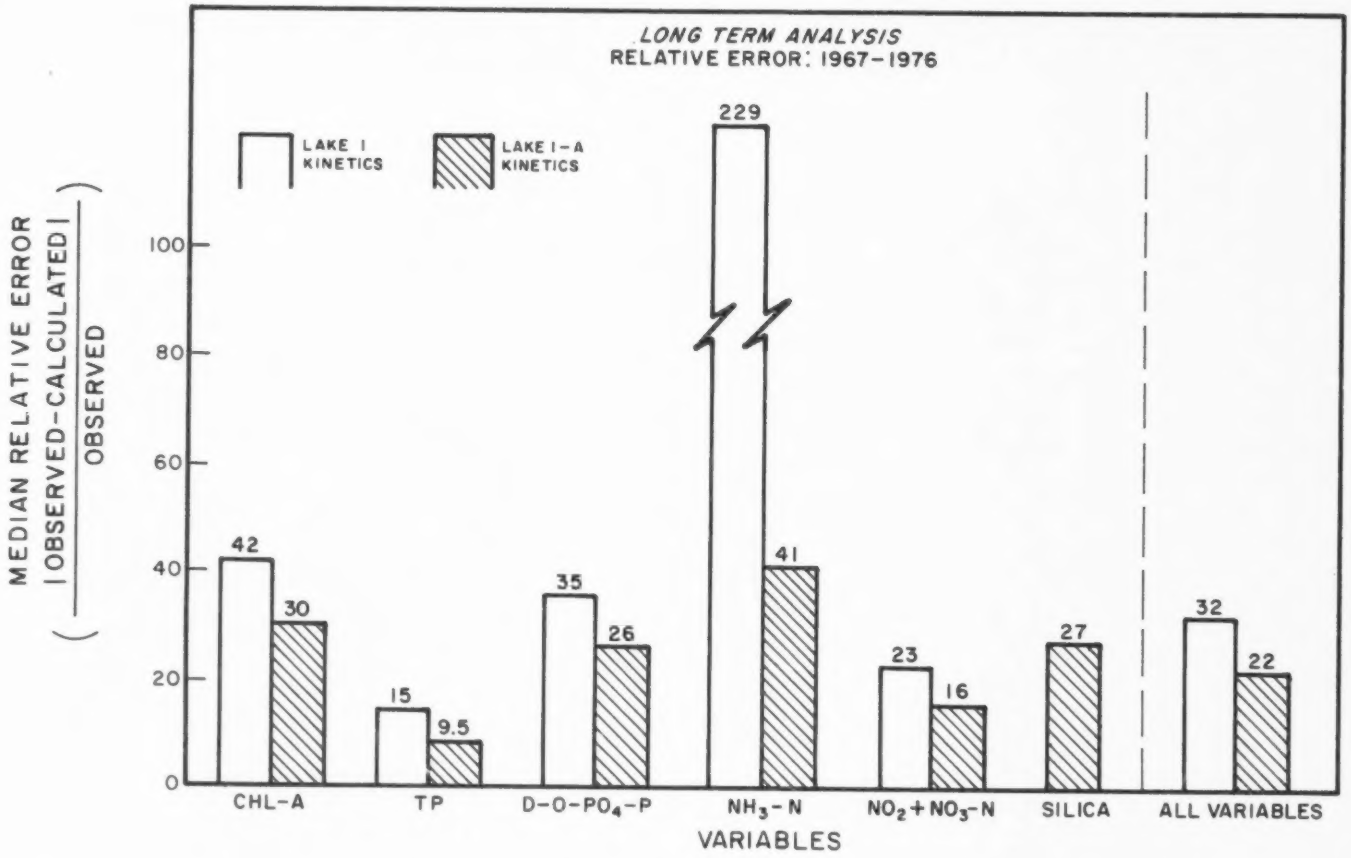


FIGURE 14. LAKE ONTARIO
MEDIAN RELATIVE ERROR, TEN YEAR ANALYSIS

THOMANN AND SEGNA 1979b

1) An urge would be created to "curve fit" model to data to improve verification statistics

2) Not all of the credibility of a model is subsumed in verification statistics

3) Good verification statistics do not necessarily imply the ability to accurately predict future water quality

4) Single measures of verification may be grasped at too readily and engineering judgment as a measure of model credibility may degenerate into "What's your median relative error?"

The advantages are:

1) Some measures, albeit imperfect ones, would be available for decision makers to assess model credibility and status

2) A basis would be provided for comparison of models

3) Some estimate could be made of changes in the state of the art of model performance

4) Modelers would be stimulated to question their model output with quantitative measures

5) A diagnostic tool would be available to determine relative improvement of a given model under more complex frameworks.

A quantitative measure of model performance, therefore, may be a mixed blessing. At the very least, the time appears appropriate to address the issue of the need and value of such measures to assess model status. It is through such discussions that perhaps some consensus can be reached on the advisability of such measures or on possible alternative means of describing the validity of water quality models.

Acknowledgments

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USE OF MODELS AS PROJECTION TOOLS

by

Robert P. Shubinski[1]

When all is said an done, the raison d'etre for mathematical models of water quality is their use as projection tools. Our concern with model verification, i.e. measuring a model's ability to simulate circumstances measured in the past, is to develop confidence in the model's ability to simulate future conditions.

This paper is an attempt to provide some definitions and guidelines that are helpful in determining the usefulness of a model for a specific goal. Analysts are often surprised when a model fails to meet the needs of a project. Frequently this could have been avoided by a careful preview to select the right model for the task at hand.

Conclusions

Personal involvement with model development and application studies over a number of years has led me to three general conclusions:

- Simplest Model. For any study the simplest feasible model should be used. The key word here is "feasible". Some problems require a complex, sophisticated model, but others do not. A good example is in the field of urban stormwater where the models STORM and SWMM are both popular. If the objective of the study is a planning level analysis of the general runoff characteristics of the system, the model STORM is a feasible model. If preliminary design of a pipe drainage system is involved, SWMM is a feasible model.

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Unfortunately, we frequently see this order reversed with the SWMM model being used with a degree of detail that is unnecessary. The result is frustration and unnecessary expense, and the analyst can come to believe that he has more information about his problem then he possesses in reality. Use of a simple model where it is feasible often keeps the analyst aware of the degree to which his judgment is crucial to the solution. It diverts him away from the trap that the model, because it is complex and wonderful, will solve his problems for him.

- Basic Relationships Model. To the extent possible, a model should be calibrated on basic physical, chemical and biological parameters. Too many models are little more than elaborate curve fitting techniques. They permit us to characterize the past behavior of a system with a good deal of accuracy, but they do not inspire confidence in our ability to use the model as a projection tool. Often it is difficult to distinguish between basic parameters and curve fitting parameters since many of our most widely used relationships have an empirical basis. However, a model that has been calibrated by adjusting Manning's coefficient or dispersion coefficients or some other appropriate parameter is always superior for projection purposes to one in which polynomial coefficients or other nonphysical descriptors have been fitted.

- Importance of Flow Modeling. Good water quality modeling requires a good solution of the flow problem. Most water quality models are driven by flow which is the principal force in moving and mixing water quality constituents. It would seem that adequately modeling the flow field would be a prerequisite to any water quality modeling, yet this is often not the case. A number of complex water quality models that describe the mixing of constitutents and the kinetics of their interaction with each other and the environment have been developed on the basis of very weak inferences of the flow field. The results of such modeling are uncertain and difficult to support.

Classes of Models

It is useful to categorize models for projection purposes into two classes. We shall call these classes "closed end models" and "open end models". From a mathematical standpoint, the former would include those problems described by elliptic partial differential equations, while the latter would include problems described by parabolic or hyperbolic partial differential equations. For our purposes here a more physical definition is useful:

- Closed End Models. These are models of systems whose response is primarily a function of the driving variables. They are essentially boundary value problems in which flow and mass continuity generally are satisfied by identity. The model is used to show how the variables within the region respond to the imposition of certain boundary values.

  An example of a closed end model is the dynamic flow and water quality problem in the bay or estuary. Water movement is controlled by the tidal boundary condition that is a primary driver and by the upstream inputs to the system. Water quality constituents are input to the system, transported about by the flow fields and its corollary dispersion, and leave the system at appropriate points. If this type of model is run for a very long period of time, it reaches a state of dynamic equilibrium in which the flow and mass inputs exactly match the flow and mass output of the system. The model is generally stable provided certain numerical inaccuracies can be disposed of. Errors in the boundary conditions show up as stable errors in the solution.

- Open End Models. This class of models is represented by the initial value problem, particularly those in which flow and mass continuity are not satisfied by identity. The end result is a solution highly dependent upon parameters in the model and certain errors are cumulative, not self-correcting.

  Some ground water models fit the open ended category. A set of initial conditions is required to start the model, and inputs and outputs must be specified by the user. Lengthy operation of such a model may result in depleting the aquifer or creating a flood. Similarly, some ecosystem models are open ended and will produce an infinite amount of biomass if operated for a long enough period of time. In other words, models of this type are not self equilibrating. They are useful for projecting future conditions to a point, but must be used with some care.

Purpose of Models

There are several rather distinct reasons why we want to use models and because of these different purposes, different model systems are required.

- Select or Screen Alternatives. Models are used in many planning programs as a tool in screening alternatives. In this type of use, we are more interested in the relative impact of alternatives than in their absolute impact, although this is not strictly the case. By and large, we use the models to decide whether or not to build a facility, the type of facility to be built, and the size it must be. The same process is carried out when dealing with nonstructural alternatives, but it is most clearly understood when discussing capital improvement projects. This is the type of problem for which long range planning models, followed by more detailed design models are often appropriate.

- System Operation. Sometimes we use a model to determine what will happen as a given system is operated. Here we are more concerned with quantitative results, particularly if the model is to be used to provide direct guidance to system operators. Long term simulation is the rule rather than the exception, and the models used may be updated from time to time as the operation of the system is observed.

- A Learning Tool. One of the unexpected benefits of modeling is its ability to teach its users how the system operates. A model cannot be used to develop "new science". Self teaching models are still in a very primitive stage at this point. However, most modelers find that repeated usage of the tools develops in them a better understanding of the system, within the constraints imposed by the assumptions in the model.

Classes of Error

Most modelers strive to determine how good their models are. That is, how well do they simulate the prototype system, and what are the sources of error that must be taken into account in evaluating model results. Generally there are four classes of error:

- Lack of Knowledge. A good model requires that its originator understand the cause and effect relationships operative in his system. Unfortunately, there are physical, chemical, and biological processes at work in water resource systems which are not so clearly understood. If they are understood in a qualitative sense, they may not be quantifiable. Hence, a major source of error in models is caused by incomplete relationships or inaccurate coefficients.

- System Changes. The idea of using a model as a projection tool implies its applicability to situations which do not yet exist. This may include changes in population, land use, waste load characteristics, and a host of other parameters. Naturally, the errors inherent in our inability to project population adequately will show up in our inability to project wasteloads and other consequences of the increase in population. Thus we must be able to project not only the results inside the model, but the initial conditions, boundary conditions, and other driving forces which determine the predictions of the model.

- Uncertainties of Nature. Many of our problems deal with natural forces in hydrology, chemistry, and biology that are uncertain as to the magnitude, timing or sequence of their occurrence. Many aspects of the hydrology, for example, are best understood in statistical terms, and the degree to which our hydrologic inputs do not reflect the "correct" sequence of events will be reflected in the model output.

- Numerical Errors. Most of our models rely on numerical analysis techniques of one type or another to produce their solution. All numerical analysis techniques by their very nature contain error terms and many have in them inherent instabilities. The model user must be cognizant of these errors and it is useful to be able to distinguish them from errors of the types cited above.

Examples and Comments

Perhaps it will be useful to take the comments so far--classes of models, purposes of models, classes of error--and discuss how these might be applicable to certain types of models. The list here is not intended to be inclusive but reflects the author's experience.

- Groundwater Models. This type of model is a good example of the open ended model. The physical system is fairly well understood although in some regions the characteristics of the aquifer itself are hard to define because they cannot be seen. Groundwater responds slowly both to pumping and pollutant inputs and modeling is oriented toward long term responses. Groundwater is modeled in an effort to solve problems of water supply and pollution control, especially those associated with TDS or salinity.

- *Streamflow Models*. Streamflow models have received a great deal of attention from analysts possibly because they are more tractable than many other problems. Our interest is usually short term since there is little effect from a long term sequence in many stream systems. Streamflow models tend to fit the category of closed end models. One danger in streamflow modeling has been that water quality standards have been over-emphasized in such work. The models themselves have been simple, and an undue reliance has been placed upon simple application of the model to achieve a preset standard.

- *River Basin Operation Models*. These models are another example of the closed end model although they are normally operated on a long term basis. They are used at both ends of the hydrologic spectrum for water supply problems, both quantity and quality, and for flood control. The most serious errors with these models normally are associated with uncertainities in the inputs.

- *Lake Quality Modeling*. These models clearly fall in the open ended category. Generally they do not satisfy mass continuity per se, and if operated for a long period of time, can predict increases or decreases in mass in the system which the analyst will recognize as inappropriate.

- *Stormwater Models*. This model class cuts across many of the lines between categories which we have drawn because stormwater models tend to be both open ended and closed ended, depending on the circumstances. Stormwater models are used to determine corrective measures for combined sewer overflows and to determine changes in the system which might occur due to land use changes, development of the watershed, or other policies of urbanization.

COMMITTEE REPORTS

The response to the basic issues presented in the preceding section was formulated by assigning workshop participants to seven Topical Area committees:

1. Wasteload Generation
2. Transport
3. Salinity/Total Dissolved Solids
4. Dissolved Oxygen/Temperature
5. Bacteria/Virus
6. Eutrophication
7. Hazardous Substances

In order to focus the committee discussions on the basic issues, the following questions were suggested:

Issue 1: Role of Models in Decision Making

What areas of agreement and/or conflict do you see in the relationship between decision maker and the use of water quality models in your topical area?

Do you think that the models have been too readily embraced by the management community or, conversely, that model results in your area have been generally ignored?

What have been your experiences with the issue of model credibility and the role of models in decision making?

Issue 2. Data Base

What is your assessment of the adequacy and reliability of the data base for water quality models in your topical area?

Can you identify any gaps or deficiencies in the data base that you presently work with? Specifically, the status of input load data, water quality and model parameters should be addressed.

Issue 3: Time and Space Scales; Kinetic Detail; Cost Effectiveness

How do you go about choosing a modeling framework in your topical area? What criteria do you use to determine time and space scales and the level of kinetic detail?

What is your assessment of the present state-of-the-art of validation of computer software in your topical area?

Do you think a "standard numerical solution" for several computer based problems should be available so that computer programs could be validated?

Issue 4: Parameter Estimation

How do you estimate the parameters in your models? What procedure do you use? What criteria do you apply to determine the credibility of the parameters?

What statistical approaches would you suggest be used in parameter estimation?

Issue 5: Measures of Verification

What procedures do you follow to calibrate and verify your models? What techniques do you use to judge the credibility of your model?

Do you think that a set of statistical techniques should be promulgated to quantitatively describe model credibility? If so, what techniques would you recommend?

Issue 6: Use of Models as Projection Tools

What criteria do you use to select the projection conditions for model simulations?

What is your assessment of the ability of your models to describe the incremental water quality changes under future design conditions?

How would you describe model credibility for systems where data do not exist (i.e. new reservoirs)?

Summary Question

Overall, how would you describe the present verification and credibility status of the models in your topical area?

Following discussions of these questions, a brief summary of the state-of-the-art of water quality modeling for each topical area was presented at a plenary session. The committees then continued deliberations individually to address the question of recommendations. The following questions were suggested to the committees to assist in the discussions or recommendations.

> What recommendations would you make to improve the usefulness of models to decision makers?
>
> What data gathering efforts are recommended to address noted deficiencies?
>
> Can? Should? guidelines be established for various problem settings for cost effective modeling studies? Are "standard solutions" required for model "validation?"
>
> Do you have any recommendations on methods for verifying models? For selecting appropriate parameters? For using models in a projection mode?

In general, the draft committee reports submitted by the committee chairmen at the close of the workshop or shortly thereafter were compiled by Hydroscience in a standard format and sent out for review by committee members. Subsequent comments were incorporated by Hydroscience and a final report resubmitted to the committee chairmen for approval. The committee state-of-the-art reports and recommendations are compiled in the following pages.

STATE-OF-THE-ART REPORT

of the

Wasteload Generation Committee

Anthony S. Donigian, Jr. - Chairman

Members

Douglas Ammon
Eugene D. Driscoll
John E. Hesson
Wayne Huber
Marshall E. Jennings
Michael L. Terstriep

Issue 1: Role of Models in Decision Making

In terms of modeling, the committee redefined wasteload generation to include the generation and delivery of nonpoint source (NPS) pollutant loads from:

- urban (stormwater, combined sewer overflows (CSO)
- agriculture
- construction
- mining
- silviculture
- other areas (rural, forest, natural background).

In general NPS models have been adequate for planning level decisions to provide overall direction and guidance to future analyses. They have been used primarily for assessment type analyses, as opposed to evaluation of alternatives. Emphasis has been on the water quantity portions of NPS models and the results have been reasonable; the water quality portions are often questionable (generally due to lack of appropriate data) but adequate to determine whether or not a problem exists and its general magnitude.

Just recently the need for models to evaluate the effects of control measures, management decisions, and best management practices (BMP's) has been recognized but adequacy of current models is uncertain. Money will likely be spent in the next few years on implementing BMP's although the ability of current models to project BMP effects is uncertain especially for the water quality portion of NPS models.

There have been mixed reactions related to model credibility. Models have been accepted in many cases where they have been properly applied (to problems for which they are appropriate) and some attempt at verification has been made. Models have not been accepted in some cases but this is often where the model has been mis-used or improperly applied.

There remain some basic limitations in current NPS models to accurately and reliably predict NPS loads in many situations.

Issue 2: Data Base

The available data base for modeling is generally inadequate and often of questionable reliability. No general data base exists that's appropriate for nonpoint sources. (This includes STORET and the University of Florida (UF) Urban Data Base.) The USGS fixed sampling stations are generally on relatively large rivers that include effects of point sources, nonpoint sources and instream effects. Much of the available information on small watersheds (e.g. in STORET and the UF data base) is end-of-pipe data that can't characterize the cause/effect relationships important to NPS pollution. However, the data can often be used in general assessments and overall planning decisions, especially when no other data exists.

Gaps/Deficiencies:

Extensive data surveys (collection programs) are needed on relatively small watersheds with preferably uniform land use to include:

- concurrent rainfall, runoff, and water quality data
- assessment of sources: rainfall quality, build-up/accumulation of pollutants
- characterization of sediments, e.g. pollutant strength, particle size, partition coefficients
- inventory/log of activities e.g. tillage/fertilizer practices in agricultural areas, construction or silviculture practices, mining activities, etc.

The data surveys should be distributed across the U.S. to represent soils, geographic and climatic conditions, and should last for an extended period (e.g. 3-5 years) depending on the specific use of the data - calibration, verification, post-audit analyses, long-term cause/effect definition. Additional documentation should exist to include maps, photos, drainage plans, sampling/analysis procedures, quality control methods, watershed characteristics, etc.

Extensive data has been collected by the USDA (ARS and SCS) on many agricultural areas across the country. An agricultural data base, similar to the UF Urban data base should be established to make the data available and accessible to the people who could use it, especially for modeling. (A new data collection program by USGS-BLM is underway on western watersheds being strip-mined.)

Issue 3: Time and Space Scales; Kinetic Detail; Cost Effectiveness

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Different time and space scales are needed depending on the problems being analyzed, the watershed behavior/response, and the model being used. Generally NPS models should be calibrated on relatively small areas (and on short time intervals) so that the measured output of the basin is due primarily to nonpoint sources. Hourly rainfall data is commonly used, but shorter time scales may be needed especially for calibration. For long-term simulation runs hourly rainfall from the National Weather Service (NWS) stations is often the only extended record available.

Kinetics are generally ignored in many NPS models, since the pollutants are assumed not to change or transform during the short residence or transport time on the surface. However, detailed agricultural runoff models that simulate soil processes may include transformations of pesticides and nutrients in the soil. The transformation interval does not usually need to be as short as the simulation interval.

The committee feels that validation of the software being used, i.e., correctness of calculational procedures, conservation of mass, adequacy of kinematic routing solutions, etc., is not often done but should be considered. For NPS process models, standard solutions may not be available, so a high quality data base should be developed as a comparison for solutions from model output.

Standard model input and corresponding output - together with program documentation - should be distributed with source decks so that the user can verify that the model is calculating correctly on his or her computer facility.

With respect to time/space scales, average annual loading models may be used for gross preliminary assessments but detailed analysis will usually require a process-oriented simulation model.

Issue 4: Parameter Estimation

Default parameters should not be used without a user being aware of the assumptions inherent in the default values. Generally, policy should be to justify the selection of all parameter values. The committee encourages the use of models with physically-based parameters that can be measured from watershed characteristics, hydrologic response and meteorologic conditions as opposed to literature values. Parameter values from nearby similar watersheds, including calibrated values can be used. However, many parameters may be based simply on calibration.

Credibility is based on a reflection of how well observed and simulated values agree using a set of parameter values that are physically reasonable and within accepted limits.

Statistical approaches are not generally used for NPS models, except to estimate sediment-pollutant relationships, and sometimes as guidance for parameter adjustments. Such statistical approaches are not widely used or accepted but might be examined for possible use.

Issue 5: Measures of Verification

The calibration procedure involves developing the best first estimate of parameters which are then adjusted as a result of comparing simulated and observed values. A reasonable water quantity (runoff) calibration is needed before attempting water quality calibrations. For models that simulate pollutants related to sediment or solids, both runoff and sediment/solids should be calibrated before proceeding to pollutant calibrations.

Split-sample calibration/verification is highly recommended. However, in data-poor situations there is a real question as to whether to calibrate on half the data and verify on the other half, or obtain the best calibration on all the observed data. In any case, credibility is based on the ability of a single set of parameters to represent the entire range of observed data. Overall model credibility can be enhanced if the model is applied by independent users, in a variety of watersheds, and for a range of events with different magnitudes. If a single parameter set can reasonably represent a wide range of events, then this is a form of verification.

If calibration is performed on a subcatchment, and the model parameters are extrapolated to the entire catchment for receiving water simulation, some assessment of the reasonableness of the entire NPS load should be made. This may need to be done in the receiving water portion.

Quantitative measures of verification are needed and model reports should always include comparison of simulated and observed data. This should be done for runoff volumes, pollutant loads, hydrographs and pollutographs. Correlations of point-to-point comparisons may not be valid, due to time shifts. For NPS pollution, mass loads are usually more appropriate for comparison than concentrations. More work is needed to specify what s specific statistical measures should be used - and are relevant - for NPS model verification.

Issue 6: Use of Models as Projection Tools

Projection conditions are generally a function of the problems to be analyzed and the questions to be answered. The model needs to be capable of representing the future conditions/alternatives to be evaluated, most likely through adjustment of parameters.

In a planning context, continuous simulation may be used to choose design conditions, and may involve the joint simulation of NPS loads and receiving water impacts. In general, detailed analyses of a runoff-quality problem should include planning level simulations using long-term rainfall records. From the resulting simulated runoff quality information, critical events can be selected that provide a desired magnitude and/or frequency of pollutant mass, concentration, duration, etc.

Current models are limited in their ability to represent incremental loads resulting from a wide range of future conditions (control measures, land use changes, management practices) due to both limitations in the data for calibration and in the model formulations. As additional data becomes available, formulations can be improved. However, in many cases, current models are the only feasible way of analyzing potential effects of future conditions i.e. models are often the only "game in town."

In situations where no data exists, reasonable values for loads can be obtained from extrapolation of parameters from other areas. There is a real question as to whether simple or complex models are most appropriate for this.

RECOMMENDATIONS

of the

Wasteload Generation Committee

Recommendations to improve use of modeling:

1. Identify the problem and the specific information to be provided by the model.
2. Select the model most appropriate to the problem and one that addresses the questions and concerns of the decision maker; use existing models to the extent possible.
3. Models are tools for aiding in decision making and should be applied by personnel with appropriate background and skills.
4. During the course of model studies, close coordination and communication should be maintained between the modeler/analyst and the decision maker.
5. Model assumptions and limitations should be clearly specified especially in relation to the conditions/ alternatives to be evaluated.
6. Emphasis should be placed on analysis and presentation of model results, especially in terms easily understood by the decision maker and relevant to his information needs.

Data Needs and Recommendations:

1. A comprehensive, high-quality data base should be established for the purposes of model testing and improvement. This should include the extensive data surveys (described in the second Issue paper) that will meet and likely exceed the needs of current models to help advance modeling state-of-the-art. Existing data does not serve this purpose.

2. The interagency agreements, such as the EPA-USGS efforts in the National Urban Runoff Program should be encouraged and expanded as a mechanism for establishing such a data base. The data should be in a form and framework where it will be readily available and accessible to the profession.

3. Current practice in urban areas does not emphasize an understanding of fundamental processes, thus data programs and associated research should be established to correct this deficiency. Source control mechanisms require this fundamental understanding.

Specific Areas for Further Investigation:

1. Erosion and sediment transport (delivery) processes.
2. Sediment-pollutant interactions.
3. Accumulation and washoff processes.
4. Subsurface movement and transport of soluble pollutants, especially in rural/agricultural areas.
5. Snowmelt quality especially in urban areas.
6. Precipitation quality.
7. Continuous monitoring of in-stream quality in conjunction with washoff studies.

STATE-OF-THE-ART REPORT

of the

Transport Systems Committee

Richard J. Callaway - Chairman

Members

John D. Ditmars	John K. Robertson
Dennis Ford	M. Llewellyn Thatcher
Gregory Han	Arthur C. Tingle
Peter F. Lagasse	R. G. Willey
John F. Paul	P. Jonathan Young

Introduction

The Tranport Systems Committee (TSC) was comprised of individuals with interests in several fields--watersheds, lakes, reservoirs, estuaries, rivers, coastal and, where applicable, the interface between these systems. Recommendations of the committee reported below are, for the most part, common to all areas in order to make the report as general and compact as possible. Readers will, of course, be aware that it is not possible to address all these systems in any great detail in so short a space and time frame.

The underlying philosophy of the TSC was that without a realistic simulation of the physical processes acting to advect and diffuse dissolved and particulate matter in whatever water body, the water quality aspects of a modeling effort would be suspect at best. This philosophy was also expressed during the meeting by the other Committees and can best be expressed by acknowledging that while the transport people (primarily hydrodynamists and/or physicists) can work on their own problems independent of water quality considerations, the reverse is not always true. It is also acknowledged that many water-quality modelers are quite competent transport modelers. Realities of the present day funding situation suggest, however, that hydrodynamic modelers would do well to join efforts with biologists, chemists, and engineers in focusing efforts toward evolution of water quality models. Some would argue that multiple use water quality modeling has arrived at the consortium stage (others will deeply regret this).

The TSC found the concept that transport model results are simply input data to water quality models useful. This concept provides a means of dealing with the two extreme generalizations that "transport modelers are not satisfied unless all details of the flow field are included in three-dimensions, with all of the proper "bells and whistles" and that "only crude transport models are necessary for water quality models, since large uncertainties exist in the chemical and biological kinetics anyway." Thus, the level of sophistication of a transport model should be determined by the sensitivity of the water quality model to transport input data and the degree of confidence required for that data.

In responding to the Issues, the Chairman has compiled the written responses of the TSC members, his own notes, and the more complete notes of Dr. P. J. Young. The TSC members reviewed and commented on the compilation. The final version incorporates their views, although in such a diverse group it would be unrealistic to assume that this represents a consensus report.

Issue 1: Role of Models in Decision Making

What areas of agreement and/or conflict do you see in the relationship between decision maker and the use of water quality models in your topical area?

It was agreed that the main obstacle in the relationship between decision makers and modelers was lack of communication. The decision maker is usually under a time constraint, political pressure, environmentalist lobbies, etc. It is doubtful if a decision will be made purely on the outcome of a modeling effort, nor is it clear that it should, considering the forces acting. Communication gaps occur from both "sides." The modeler sometimes oversells his product, through an enthusiasm for his own work; if the decision maker goes along with the modeling effort on that basis and is burned, it may be a long time before he accepts once again a modeling output without considerable skepticism. The modeler, too, is vulnerable in that the decision maker may misinterpret or misapply his results.

The solution to the communication problem lies in educating the decision maker with regard to the constraints, assumptions, reliability, and realism of modeling as only one tool available to him. On the other hand, the modeler should be aware of the policy involved and, where necessary, direct the model to a specific application that the decision maker requires. The dual role implied above is not going to be solved at a workshop between modelers and decision makers, but will require continuous interaction between two very dissimilar groups.

Finally, the decision maker often seeks answers to questions for which no adequate model exists. Too often modelers have applied inappropriate models (of transport mechanisms, at least) in an effort to obtain quantitative results. Examples abound.

Do you think that the models have been too readily embraced by the management community or, conversely, that model results in your area have been generally ignored?

The TSC members were unanimous in that inexperienced management usually accepts modeling results. Indeed, they are too often uncritically accepted and with little appreciation for the limitations of the analysis (discussed above). There was indicated a human tendency to accept more readily results when they are in support of a, perhaps, preconceived judgment. The experienced decision maker, on the other hand, while accepting modeling efforts, usually does so with a healthy skepticism; it is not infrequently the case that he knows what questions to ask of the modeler. The best overall results occur when there is an open search for the real meaning of the results and a non-defensive response by the modeler.

What have been your experiences with the issue of model credibility and the role of models in decision making?

Modeling has undergone a series of hill-and-valley traumas, the valleys caused by oversell of the product followed by trivial, misleading, or downright wrong answers. Credibility has fluctuated similarly from blind acceptance to a state of not even wanting to hear the word "model." At this stage, we seem to be mounting another hill and we should make use of past experience and mistakes to regender credibility. The enormous complexity of today's environmental issues make model use an absolute requirement, if Federal agencies responsible for water resources are to reach objectives imposed by the law makers.

Issue 2: Data Base

What is your assessment of the adequacy and reliability of the data base for water quality models in your topical area?

Can you identify any gaps or deficincies in the data base that you presently work with? Specifically, the status of input load data, water quality, and model parameters should be addressed.

The TSC response to this question was mixed. Those who found the data base adequate and reliable were in a position of specifying, collecting, processing, and analyzing their own data. This leads to the conjecture that they found the existing data base inadequate and unreliable, hence the spawning of their own data base. Those who found the data base inadequate at the outset, either made do with what was available or conducted interpolation-extrapolation field surveys.

The reliability of such time-honored data collectors as the USGS was generally reliable; problems arise, however, in the coverage available, the time lag in obtaining the data, and the costs involved. The National Ocean Survey tidal elevation data are not consistently reliable, and datum elevations are not always available. A serious time lag is involved in obtaining NOS data in a suitable format as a result of understaffing and because NOS is not primarily a data retrieval organization.

Synoptic data sets for model calibration and verification are virtually absent for hydrological systems. Climatological data sets are more intensive in a time-series sense but also are sparse in areal coverage. (Climatological calibration raises a whole new set of related quations.) The problem of open boundary data, particularly in coastal areas, is one of expense and difficulty in measurements. Nearshore data are often lacking in coastal areas and in large lakes simply because vessel masters are sensitive to keel to bottom depths and because oceanographers have traditionally had strong offshore interests.

The dissatisfaction with the existing data base stems largely from the fact that the data set (e.g., USGS stream gauge measurements) were not set up with a modeling effort in mind; rather, commitments to some other mandate were made years before modeling became _de rigueur_. Said another way, funding agencies are more willing to support monitoring rather than research.

Modeling of sediment transport (suspended and settleable) suffers from a lack of quantification which results from inability to specify correctly settling velocities, critical erosion velocities, and a general lack of understanding of the physics and mechanisms involved in sediment transport processes. Where toxic materials are sorbed into particulates, this lack is critical to an understanding of the hazardous substance problem. Basic research on hydrodynamic models with field investigation feedback is necessary if we are to solve these fundamental basic research problems.

Issue 3: Time and Space Scales, Kinetic Detail, Cost Effectiveness

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How do you go about choosing a modeling framework in your topical area? What criteria do you use to determine time and space scales and the level of kinetic detail?

Response to this question was rather vague. For some cases, a steady-state, one-box model may be perfectly justified; e.g., geochemists usually are concerned with time scales of centuries, kinetic modelers with seconds. Space scales vary with the type of problem, computer facility, computer budget, and the physics of the system-- i.e., are we dealing with a well-mixed system, or do we need to simulate a multi-level or vertically continuous system? If a variable grid is employed (e.g., finite element methods), then spatial detail near a source would be desirable, with a larger grid spacing at distance from the source.

The Water Quality (WQ) Committees will address in more detail the questions of kinetics; the TSC concern is to sufficiently detail the transport processes on which the WQ topics will piggy-back. Examination of the transport equation (advective-diffusion equation, dispersion equation, etc.) reveals a galaxie of approaches as to the terms employed, the bulk coefficients used to gloss over ignorance and/or lack of measurements, etc. It is worth noting that integrations in time and space of the transport equations yield simple models with coefficients that reflect all the details ignored and that are not universal, while less highly integrated forms yield complex models with more physically meaningful coefficients and require small time and space steps. The dichotomy is that simple models may be in terms of long time scales and averaged space scales that decision makers like, but have no predictive capability and that complex models may have better predictive capabilities, but on scales of meters and seconds.

At any rate, the modeling framework must proceed hand-in-hand with the objectives of the study--perhaps as set forth quite sketchily by a decision maker--budget and time constraints, and the projected field effort.

The Chairman's experience with a variety of commercial contracts and university grants has been that hydrodynamical models, per se, don't sell at the headquarters level unless strongly coupled with a water quality objective. Given the priorities involved and the dollars available, this is probably realistic, but does not respond to the question of which federal agency will support pure hydrodynamic--related research.

What is your assessment of the present state of the art of validation of computer software in your topical area?

Probably some workshop attendees have been guilty, at one time or another, of taking a model off the shelf and running it. If a canned model is to be used in a major decision making effort (which may end up in court), one must be completely satisfied with the documentation and coding of the model, its assumptions, limitations, areas of applicability, etc. The "bug"-free model is a rarity if the program listing consists of several thousand lines. The recent lesson provided by the NRC shutting down of five nuclear power plants is a case in point.

Do you think a "standard numerical solution" for several computer based problems should be available so that computer programs could be validated?

The TSC was quite happy with this question, since they quickly and unanimously converged on the opinion that a "standard numerical solution" had a peculiar dreamlike quality. If the exact same differential equations were employed, and if the same boundary conditions were employed, etc., then differences between solutions would be a function of the numerical techniques employed--which was the point of the question, presumably. Numerical techniques are sometimes a personal choice--i.e., finite differences vs. finite element methods--and do not necessarily converge at the same rate.

It was felt that more important would be a "standard" river or a lake or estuary sufficiently instrumented and data processed to permit verification of one's software. (It is duly noted that not all commenters on this last sentence were entirely happy with it.)

Issue 4: Parameter Estimation

How do you estimate the parameters in your models? What procedure do you use? What criteria do you apply to determine the credibility of the parameters?

The general procedure employed was based on knowing (from experience) what range of values to anticipate and consequent simulation over the range. Where only a few parameters are involved, this is not a difficult undertaking but may involve many computer runs. Where many parameters are used, sensitivity analysis should be achieved as, e.g., employed by Tomovic (1963)*. The idea is to relate the change in a system component as a result of change in some other variable, flux or parameter.

*Tomovic, R. 1963. Sensitivity analysis of dynamic systems. McGraw-Hill, New York. 142 pp.

What statistical approaches would you suggest be used in parameter estimation?

Typical responses to this were somewhat unsophisticated relying primarily in root mean square computations. Residual plots and sums of errors criteria are used, but others felt that statistical verification either didn't exist or was an art form.

During the general discussion period of all Committees, it was brought out that the meteorologists have been using statistical methods routinely for a number of years and have developed a subculture devoted to statistical forecasting, skill scores, data smoothing, verification, etc. Water quality modelers, on the other hand, have avoided this approach successfully to date, but will have to become involved as more and more court actions are carried out.

Issue 5: Measures of Verification

What procedures do you follow to calibrate and verify your models? What techniques do you use to judge the credibility of your model?

For some simple systems, numerical transport models are amenable to comparison with classical analytical solutions. As the complexity of the system simulated increases (non-linearity, multi-dimensions), analytical solutions are not usually available. Residual values (observed minus predicted) need to be examined at several locations within a closed system. Assuming specified boundary conditions, the interior solutions will differ from observed values as a function of the solution method, interior environmental conditions, degree or presence of discontinuities, etc. Plotted comparisons of residuals, while not necessarily quantitative, give the experienced analyst a good idea as to the validity of the simulation. The goodness of fit may not be obvious to the decision maker, so it behooves the analyst to discuss the verification procedures employed.

Of course, true verification is obtained after fine-tuning the model to a given situation and then running it and comparing it against another set of input and boundary conditions. Difficulties arise when a given parameter is not expressed as a function of a measureable physical quality of, say, velocity or hydraulic radius.

In some situations Monte-Carlo techniques can be used (e.g., for reservoir modeling) to give confidence intervals.

Do you think that a set of statistical techniques should be promulgated to quantitatively describe model credibility? If so, what techniques would you recommend?

"Promulgation" turned off the TSC audience. Depending on the model and the parameter to be verified, a certain standard statistic may show results that are biased - either to the good or bad. Choice of an appropriate set of statistics is best left to the analyst who knows the data set and its reliability, the system, the model, and the constraints involved. For some, statistical analysis was best relegated to self checking or guidelines, not necessarily for publication.

Since the verification data itself may contain considerable noise, imposition of statistics is not as simple as it may appear. Statistical techniques may mask serious errors in some areas.

The variety of statistics available is too great to recommend a list of techniques. Many WQ modelers are not necessarily into statistics beyond root mean squares and the t-test. Meteorologists have much to teach us (as they have in the past in the hydrodynamics scene).

There was, in general, a rather uncomfortable feeling about the use of statistics as part and parcel of the transport analysis; it is felt that there was a natural reluctance to bite the statistics bullet, but an acknowledgment on the part of potential courtroom drama participants that the time of defending a given analysis with statistics has, for better or worse, arrived.

Issue 6: Use of Models as Projection Tools

What criteria do you use to select the projection conditions for model simulations?

When working with a water quality modeler, the transport specialist must have a thorough knowledge of just what are the WQ objectives in terms of detail required and what degree of uncertainity in the transport input the modeler is willing to accept. Put in terms of a commercial application--what does the client want? This is not to be confused with getting what the client wants but in determining the simplest method of evaluating a given situation in terms of client need. Projection conditions, then, are defined by the client's objectives and desired alternatives.

What is your assessment of the ability of your models to describe incremental water quality changes under future design conditions?

Responses varied to this question. For instance, it was suggested that errors in the receiving stream model may be far less than those of the input data set, and the errors in transport may be far less than kinetics of constituents. If the physics are well represented, then one-dimensional model simulations would be adequate; however, few post-audit cases have been documented.

In reservoir models, there still is an inability to represent the onset of stratification, indicating a need for basic research on this phenomenon.

How would you describe model credibility for systems where data do not exist (i.e., new reservoirs)?

See Part 1 of this Issue regarding input data.

Committee members were skeptical for the most part, largely because there have been few cases where there has been a post-audit attempt. In the reservoir situation, similarly sized reservoirs and watersheds are studied with a view toward predicting outcomes for new reservoirs. Unfortunately, reservoirs take a long time to be constructed and put into operation, and the impetus to go back and check calculations is lost as new generations of engineers come on line.

River and/or aqueduct simulations are generally amenable to open-channel hydraulic solutions; problems still will exist with regard to water quality, weed growth, etc.

RECOMMENDATIONS

# of the

Transport Systems Committee

What recommendations would you make to improve the usefulness of models to decision makers?

Based on past experiences and as discussed in Issue 1, the credibility of modeling in the eyes of the decision makers has suffered because of a lack of understanding on their part to the limitations of models, and also because the modeler has not always represented the model well. The decision makers' expectations having been dashed, they sought other-than-model solutions to political/environmental problems of mind-boggling complexity. The inherent non-linearity and many-bodied nature of the problems points directly to a mathematical analysis of some sort. Mathematical analysis suggests a model, be it linear programming or hydrodynamical in nature. That being the case, the decision maker is bound to use models if he is to be effective. Therefore, he must either be experienced in modeling himself (not necessarily a sufficient condition) or be capable of appreciation of model use. Eventually, he will have to know what questions to ask of the model.

The modeler is not absolved of responsibility in the education-technology-transfer process between computer output and the decision maker. He must anticipate the questions likely to be asked and point out areas that the model indicates should be examined (but were not identified initially).

The discussion above is rather obvious and may be platitude prone, but for optimum utilization of the skills of modelers and the benefits of modeling there is required an interaction between two very different levels of achievement--management and science.

What data gathering efforts are recommended to address noted deficiencies?

With some notable exceptions, most modelers are condemned to use "other people's data," data not usually gathered for a modeling effort. The TSC was unanimous in the opinion that modelers should be involved at the initiation of any data gathering event, i.e., if a model is likely to evolve, modelers should get involved. The modelers' advice should be sought when choosing the location of measurement sites based, when feasible, on preliminary model runs. The objectives of this effort are to minimize sampling time and scope and the number of stations required. Because time-series data will be required and because of the logistic problems involved, care must be taken to select these stations with a minimum of hassle to the budget and the body.

Can? Should? guidelines be established for various problem settings for cost effective modeling studies? Are "standard solutions" required for model "validation"?

No. No.

Do you have any recommendations on methods for verifying models? For selecting appropriate parameters? For using models in a projection mode?

Since this is so model dependent, the question degenerates into a list of references. Leendertse's work in Jamaica Bay, for instance, may be cited.

Overall, how would you describe the present verification and credibility status of the models in your topical area?

With regard to estuarine transport processes, the TSC recommended adoption of the report by Kinsman, et al.* The following sentence from the preface responds to the above question: "It was the very strong consensus of the group that recent data show many of our previous ideas of estuarine transport processes to be overly simplistic and that a greater level of sophistication of our understanding of these processes is required, not only for a significant scientific advancement, but also for effective environmental protection and management." The report of the Kinsman study makes many pertinent recommendations on verification, flux term investigation, small and large scale experiments, etc. Their arguments will not be repeated here; suffice it to say that the majority of their recommendations also apply in part to reservoir and large lake modeling.

We close this section with another quote regarding estuary models from Kinsman, et al.: "No model which has not been both verified and tested can be considered anything but 'work in progress'. It is something of a scandal that none of the

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*Kinsman, B., J.R. Schubel, M.J. Bowman, H.H. Carter, A. Okubo, D.W. Pritchard, and R.E. Wilson. 1977. Transport processes in estuaries: Recommendations for research. Marine Sci. Center, SUNY Spec. Rept. No. 6, Ref. 77-2, 21 pp.

'models' we now have has been either verified or tested in its complete form. The data with which to do so have never been taken."

What overall recommendations would you make regarding water quality model verification? What needs in this area of verification do you perceive to be most critical in the future? What specific programs would you suggest?

No one definition of "verification" is possible when so many variables are at play in the transport-WQ modeling business. Rather, measures of model sensitivity and/or "verification" need be reported with reference to specific parameters and to specific water bodies. Therefore, we recommend that existing state-of-the-art and evolving water quality models be examined to determine the sensitivity of the model results to transport input parameters. This is because, while WQ modelers do a lot of sensitivity checking on most parameters, little has been done in transport parameters and, for certain model applications, the entire model may be transport driven.

Verification for different systems will differ. For instance, in a very broad sense, stage and flow rates may suffice for rivers; tracer distributions for reservoirs; salinity distribution (vertical and horizontal), tidal heights, velocity profiles (vertical and cross-stream) and tracer distribution for estuaries; salinity distribution, fixed-point velocities, total transport, and storm surge elevations for coastal areas. As part of these generalities, it is noted that verification of the same transport system may differ with the purpose of the WQ model using the transport input.

In reservoir and lake modeling, further research on stratified flow, turbulence, and vertical transfer coefficients is required. Formulation of water quality models will require compatibility of hydrodynamic time and length scales and water quality scales.

Satellite and remote sensing data should be used in conjunction with ground truth data. Physical hydraulic models should be used where possible; moveable-bed models should be of considerable interest in bed-load transport problems in estuary mouths. Features are observable in small-scale models that cannot be extrapolated from field data and may not be replicated in mathematical models indicating adjustment of the grid or an incomplete mathematical/physical analysis.

Of prime concern in many applied problems, is our present inability to measure and model sediment transport satisfactorily. Assuming that many toxic substances will be transported in settleable or suspended particular phase, it behooves the analyst to address this very difficult problem. The nature of the attack indicated is one of basic research; field measurements are notable by their absence; the pure physics of the apparently rather simple processes is also lacking.

The TSC was unanimous in the opinion that extensive data sets are needed in a variety of settings. Using estuaries as an example, it is required to fund intensive data gathering programs on all types of estuaries, including fiords. Logistically, it was pointed out that the Yaquina Estuary in Oregon is one that can be sampled from a small boat from freshwater to the ocean in a day. Admittedly a somewhat selfserving example on the part of the Chairman, it is in fact a model of the larger Chesapeake and Delaware systems. Since it varies seasonally from well-mixed to stratified (Hansen and Rattray 1-3 classification), it could provide a wealth of information on a small scale that could be extrapolated to larger, more important systems. San Diego Bay was also indicated as a tractable system for testing certain aspects of transport computational schemes in embayments.

The problem of funding was raised throughout TSC deliberations. Pure research items, such as turbulence-diffusion mechanisms, were indicated as an NSF-type area. Intensive data gathering efforts in estuaries are indicated as, at least, joint NOAA-EPA efforts. These efforts must not be designed by transport specialists only, however, since WQ problems are, in the final analysis, of prime concern.

We submit that agencies supporting modeling studies should require "verification" of transport models in terms of the particular system studied. This can be accomplished by breaking out a portion of a budget for field programs after careful consideration of the constitution of the final product. Where appropriate, model verification activities by parties independent of a particular model development might be undertaken.

Finally, the subject of statistical verification should be pursued intensively. Although there was an indication of a general audience reaction against the unfamiliar, it should prove to be a satisfying endeavor in the future since one will be able to quantify just how good (or bad) ones effort has been. If the direction is away from a battle of coefficients toward an understanding of the system, then the statistical approach cannot help but be beneficial. As far as funding agencies are concerned, they should begin thinking about how best to exploit the possibilities (not at all obvious at this stage) since they can expect to have to pay for it.

STATE-OF-THE-ART REPORT

of the

Salinity/TDS Committee

Louis A. Beck - Chairman

Members

Tze-Wen Chi	Robert P. Shubinski
William J. Grenney	Richard Tortoriello
Austin Nelson	George H. Ward

Issue 1: Role of Models in Decision Making

The committee felt that too often models have been employed for decision-specific problems; once the decision is made, further "model" development is terminated. In many instances, model development and verification should be a long-term program.

Management tends to blindly accept modeling results as scientific and quantitative when the results agree with their preconceived views. However, management questions results when they disagree. A more tempered, less extreme view is needed. Occasionally political decision makers feel constrained by modeling. Perhaps because of this, some decision makers are resistive to the use of models. At the same time, modelers should recognize there are other political or socio-economic factors that bear on management decisions.

Good judgment is essential in selecting a model appropriate to the problem at hand. Many factors should be considered and the mere availability of a computer code is not an appropriate criterion of selection by itself.

Issue 2: Data Base

There are probably more data available for salinity from surface waters than for most other parameters. Nonetheless, more data, particularly over long periods of time are required.

In estuaries, programs of long-term routine monitoring as well as intensive short-term space-time studies are needed. For wetlands, available data is practically nonexistent. Fairly good salinity measurements are available for inland surface waters over large geographical areas. There is a need, however, for data on specific ions, localized conditions, and salinity loading functions for agricultural and natural processes, especially in the arid west.

There is a lack of data on the intrusion of salinity into groundwater, whether of oceanic or geological origin. Although some data on groundwater salinity is available, it is not collected for developing a predictive tool, and therefore is nonspecific or lacking important ancillary measurements.

Issue 3: Time and Space Scales; Kinetic Detail; Cost Effectiveness

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Salinity responses typically exhibit long space and time scales in comparison with other parameters, both in surface waters and groundwater. This should be recognized in implementing data programs as well as in verifying models. This has important consequences on system characteristics, requisite data resolution, computational demands, as well as the dimensions of the problem at hand.

In inland, particularly arid regions, the state-of-the-art of model verification is behind the needs and questions being posed by management.

It is the responsibility of the agency or engineer applying a model to evaluate the model he is using for correctness of code, numerical accuracy, and appropriateness of application.

Issue 4: Parameter Estimation

Salinity may be considered a conservative substance for dilute concentrations in inland waters and also in estuaries where it is an excellent variable for estimating dispersion.

For inland systems, both surface and groundwater, the components of TDS may be subject to kinetics as well as effects of other constituents (such as pH, TSS, etc.). This is particularly true where high concentrations occur in the arid west.

Issue 5: Measures of Verification

The committee felt that verification is achieved by subjective judgement and visual comparison of model results with observed data.

Statistical techniques should be used but not promulgated. One should be free to adopt statistics appropriate to his need. Statistical techniques should also be applied to analysis of the data, especially confidence bounds and reliability, prior to its application in model validation. Because salinity occasionally has a good data base (especially for inland waters of the arid west) and simple kinetics, salinity could be a good parameter for the development and testing of statistical verification techniques.

Issue 6: Use of Models as Projection Tools

The committee felt that selection of projection conditions is dictated by the specifics of the problem and the range of conditions important to the system. It was also felt that salinity models are generally reliable in predicting incremental water quality changes under future design conditions due to the conservative nature of salinity, but this is highly contingent upon the specific situation.

RECOMMENDATIONS

of the

Salinity/TDS Committee

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1. In order to improve the usefulness of models to decision makers, there should be a close working relationship between the modeler and the decision-maker. Presentation of model results to a decision-maker should include the reliability of the prediction and, where possible, confidence limits. Demonstration of model response (i.e., sensitivity analyses) can be very useful to decision-makers.

2. A greater effort in model development for groundwater is needed.

3. The hydrodynamic/transport mechanisms need better formulation for many systems, e.g. groundwater flow, or the density circulation of estuaries. Related to this, better data on hydrodynamics/transport are needed.

4. It is important that modelers work more closely with data collectors, perhaps participating in the program where possible. One example of data inadequacy is the definition of the boundary condition at the mouth of an estuary, which is frequently assumed to be at a constant oceanic value but may be variable and require adequate monitoring.

5. The committee strongly urges that no standard guidelines for cost-effective modeling studies be promulgated. Judgment of the modeler is a very important aspect of the modeling effort and "standards" tend to reduce or eliminate this judgment. At the same time, management should not be expected to re-develop a model for each new application.

6. Verification in the past has been largely qualitative. The committee recommends a greater application of quantitative measures, though it does not think any specific statistical test should be recommended.

7. Overall, the committee feels that development is needed in four areas of application, with varying requirements and methods:

(1) Coastal Surface Waters

The most common and best developed area is the estuary, in which salinity is a parameter of central importance. The significance of coastal wetlands is now better recognized; these systems will require models, some of which are presently under development.

(2) Coastal Groundwater

Modeling is often done for salinity intrusion and probably basic relationships are generally understood.

(3) Inland Surface Waters

Modeling is done often but there are some serious unknowns, such as salinity losses in reservoirs and kinetics of specific ions in streams.

(4) Inland Groundwater

This area is least commonly modeled and much more research needs to be done in the unsaturated zone.

STATE-OF-THE-ART REPORT

of the

Dissolved Oxygen/Temperature Committee

Clarence Velz - Chairman

Members

Joe M. Dietzel
C. S. Fang
James M. Greenfield
Clark C. K. Liu
John T. Marlar
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Peter G. Robertson
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Introduction

Our committee was composed of modelers working in government, academia, and private practice, and even though there was considerable discussion during the deliberation of the issues, there was a surprising consensus of opinion. This gives us cause to believe this report reflects a relatively accurate assessment of the state-of-the-art in DO/TEMP modeling.

The committee wishes to acknowledge the fact that because of the limited time available for deliberation, our discussion necessarily focused on dissolved oxygen modeling as applied to specific water-courses. However, since the committee believes that much of the content of that discussion applies equally to temperature modeling, the interchangeability of the statements is reflected throughout this report by the use of the term "DO/TEMP."

The general findings by the committee on the state-of-the-art of DO/TEMP modeling are summarized as follows:

1. The committee agrees that the conceptual framework for DO/TEMP modeling is well founded scientifically, and that with proper application it should provide a reasonably accurate vehicle for predictive analysis. The conceptual framework as currently utilized is structured in either one, two, or three dimensions using either steady state or time variable assumptions.

Application of the framework to DO/TEMP problems is relatively easily accomplished using readily available computer programs.

2. The committee agrees that our understanding of what model parameters are important and our technical ability to obtain valid field measurements of those parameters is reasonably well advanced; however, these principles are not universally applied.

3. The committee agrees that some shortcomings exist in our current practice of DO/TEMP modeling. First, current modeling frameworks do not facilitate quantification of the random component of DO/TEMP data. In certain instances where a large random component exists, ability to forecast reliably may be impaired. Second, questions of model limitation and sensitivity may not be addressed in sufficient detail by modelers to allow the decision maker a chance to evaluate the uncertainties inherent in the projection analysis. This failure may be due in part to the inability of modelers to make these assessments themselves. Third, the accuracy of current mathematical equations to predict the reaeration rate in a watercourse is somewhat unsatisfactory and use of in-situ gas tracer techniques developed by Tsivoglou is encouraged. Fourth, there is a tendency within the modeling community to use any available data, including monitoring type data, for specific model development. Development of reliable predictive assessments of decision alternatives necessitates intensive snyoptic-type data collected in the specific watercourse being modeled.

The committee's assessment of the specific issues comprising this state-of-the-art report is presented below.

Issue 1: Role of Models in Decision Making

The attitude of decision makers toward using modeling results in the decision making process varies widely from enthusiastic acceptance to outright mistrust and rejection. The range in attitudes is explained in part by the prior track record of modelers to provide an analysis sufficiently defensible to withstand legal challenge, in part by how the decision maker perceives his own technical understanding of the issues, in part by how clearly and understandably the analyst presents his findings to the decision maker, in part by the analysts' ability to present demonstrable proof the model results are correct, and in part by the amount of time available to do the required analysis before a decision must be made. It is the committee's observation that administrative conflicts normally result more from interpretation of model results or comparisons of model results with standards, rather than from issues related to model selection. In short, modeling credibility lies more with the analyst than with the computer program which was used.

The committee agrees that the level of sophistication of specific case DO/TEMP models should be the minimum required to include not only the principal phenomena but the principal factors encompassing alternative decision analysis. The level of sophistication required should be determined on a case by case basis.

The modeler serves four principal functions in the decision making process. First, he translates the environmental issues into a program of investigation. Development of the program includes analysis of existing data and literature and consultation with people knowledgeable with the specific environmental issues. Second, he selects the appropriate conceptual framework for modeling the system such that the issues can be addressed forthrightly at the minimum level of sophistication necessary to make technically sound evaluations. Third, he oversees and participates in data collection and analysis. Fourth, he provides technical guidance in interpreting the results, in defining the confidence limits of the results, and in insuring the administrator is cognizant, within the limits of scientific understanding, of the environmental consequence of his decision.

Issue 2. Data Base

The principal issue related to the data base for DO/TEMP models is the need for intensive synoptic-type data collection surveys. The members of the committee concur that the foundation of acceptable model calibration and verification lies in a well planned data collection program, and that compromises in data collection can have a significantly adverse effect on the ultimate achievement of a reliable analytical tool. Intensive synoptic-type surveys require a substantial, well organized and trained staff of field and laboratory personnel and require a great deal of preliminary work and planning.

Since the objective of a water quality modeling study is to identify cause effect relationships, acquisition of an appropriate data base assumes great importance. Three factors should govern the design of the data acquisition program. First, sampling should be conducted over a short time interval such that a comprehensive "snap-shot" of the water quality and loading functions of the watercourse is obtained. In tidal systems, this requires slack water sampling supplemented where appropriate with selected time series data. The sampling stations should be located at intervals sufficient to elucidate the salient features of the DO/TEMP profile as well as at locations upstream of all significant point sources and tributaries. Second, the sampling frequency should not only be consistent with the time scale of the DO/TEMP model but also be consistent with the natural variability of the system. Diurnal measurements should be made at those locations where hourly variations in DO/TEMP are expected. Third, the sampling program should include direct measurement of state variables, rate constants and other physical factors that influence the DO/TEMP balance in specific areas. The state variables include, but are not necessarily limited to, long term BOD, DO, TEMP, nutrient concentrations, salinity pH, chlorophyll, etc. The rate constants include, but are not necessarily limited to, deoxygenation, reaeration, ammonia oxidation (where appropriate), photosynthesis/respiration (where appropriate), benthic oxygen demand (where appropriate), etc. The physical factors include, but are not necessarily limited to, streamflow, time of travel, tidal currents, channel morphology water depth and its change as a function of flow, meteorological parameters, etc. Wastewater flows must also be monitored for pertinent characteristics.

As noted above, good synoptic data collection of an intensive nature is an essential requirement for the application of applying micro-scale models. For the purposes of macroscale models, and for determining recurrence intervals, the data base should include a well designed long-term component.

Issue 3: Time and Space Scales Kinetic Detail; Cost Effectiveness

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DO/TEMP models must be consistent in their time and space scales with the phenomena being simulated. For example, simulation of the diurnal variation in DO resulting from carbon fixa tion and metabolism in phytoplankton requires the use of a time scale equivalent to fractions of an hour. Modeling frameworks set in different time scales may be required to address efficiently water quality issues related to mean daily or seasonal limitations for the specific watercourse under investigation. There is a misconception, however, that because seasonal changes in water quality occur, it is essential to formulate a time variable model to simulate instantaneous responses throughout the year. To do so requires exceedingly complex mathematical solution techniques and voluminous data that is not realistically attained from laboratory and field measurements. In the end, simplifying assumptions are necessary for solving the complex mathematics and for reducing the data needs. The net result is a model of questionable reliability and utility. The trade off, on the other hand, is to formulate a steady-state model to simulate the critical seasonal responses such that the mathematical complexity and input data needs are reduced dramatically. In the end, fewer simplifying assumptions are needed with the net result being a model of more reliability and utility. The cost effectiveness of such an approach is obvious. Regardless of the timeframe selected, however, the state-of-the-art of DO/TEMP modeling is well advanced.

Spatially, one, two, and three-dimensional DO/TEMP models are currently available. Here again, selection of the space scale must be consistent with the watercourse and phenomena being simulated. For example, while one-dimensional models are the most widely used in free flowing systems, their use is usually not appropriate for simulating phenomena in lakes, embayments, estuaries, or coastal waters. Numerical solution techniques developed over the last twenty years have provided the necessary tools for dealing with these more complex systems.

Undue kinetic detail is seen by this committee as a stumbling block to the effective use of DO/TEMP models as decision making tools. If a phenomenon is expected to impart a significant change in the DO/TEMP budget, then kinetic detail appropriate to simulating that phenomenon is usually warranted, as for example in simulating photosynthesis in eutrophic waterbodies. Otherwise, kinetic detail should be maintained at the minimum required to adequately reproduce the primary state variable interactions.

Existing computer programs for DO/TEMP models are generally efficient and cost effective. A standard numerical solution for different classes of problems appears to be a good idea. Such solutions would provide a benchmark by which analysts could evaluate the accuracy and cost effectiveness of a particular model. A standard numerical solution would also have the advantage of providing a useful tool for evaluating new programs and solution techniques. However, the committee feels the state-of-the-art has not advanced sufficiently to allow this approach to be implemented at this time.

Issue 4: Parameter Estimation - Calibration

Model calibration serves two important functions. First, in many instances it is the only procedure available to estimate the in-situ reaction rates for the individual components of the DO/TEMP budget. Second, it provides the modeler the first opportunity to perform a sensitivity analysis on the components of the DO/TEMP budget. Performing a preliminary sensitivity analysis at this stage permits the data acquisition program to be modified if necessary. Needless to say, selection of the significant components for inclusion in the specific case DO/TEMP model as well as estimation of the corresponding in-situ reaction rates must be determined for each watercourse using data generated from intensive synoptic surveys as well as from other specialized studies conducted on that watercourse. The practice of using reaction rates or reaeration rates taken from the literature must be discouraged unless it is demonstrated first that either the DO/TEMP budget is insensitive to the rate used or the predicted response tracks the observed response reasonably well.

As noted above, the committee is in agreement that parameter estimation for dissolved oxygen models should be accomplished through independent measurements wherever possible. Calibration should provide the vehicle whereby parameters are tuned to more accurately represent the variability of the parameters under different hydrologic and meteorologic conditions. The accuracy and credibility of the model is generally enhanced by keeping the number of parameters to the minimum required.

Selected comments and conclusions of the committee with regard to parameter estimation issues are:

1. Good time-of-travel estimates and channel geometry are essential in river systems, particularly in small streams.

2. Direct reaeration measurements using methods such as those described by Tsivoglou or Rathbun are particularly valuable and use of them should be encouraged.

3. Benthal oxygen demand measurements are best measured in-situ.

4. In developing a steady state DO model for a biologically active water body, the model parameter for photosynthesis/respiration requires careful evaluation. Or, alternatively, this term may be separated from analysis by simultaneous modification of both the mathematical formulation of the model and the data used in its verification.

5. In cases where parameter estimates depart significantly from literature values, the source of the parameter estimate should be documented. Measurements or derivations from first principles are the preferred methods of documenting these cases.

6. In preparing reports the modeling community should present tabular summaries of model parameters and, where appropriate, time histories of model parameters.

Issue 5: Measure of Verification

The committee agrees the most rigorous test of verification of a model is to demonstrate that phenomena predicted by the model actually occur under the conditions and at the locations observed in the field.

The committee also agrees another way to demonstrate verification of a DO/TEMP model is to have a calibrated model track an independent set of observed data such that good agreement is achieved throughout the profile. The data used for verification in this case must be derived from intensive synoptic surveys conducted under stable hydrologic and meteorologic conditions different from those used for calibration.

The committee agrees furthermore that statistical analysis can be a valuable tool for quantifying the "goodness of fit" between the observed and predicted profiles, but the state-of-the-art of DO/TEMP modeling is not yet advanced enough to allow promulgation of "goodness of fit" standards.

Sensitivity analyses are valuable adjuncts to verification. Since all state variables, rate constants, and physical parameters do not have the same order of magnitude impact on the modeling projections, the sensitivity analysis provides the modeler with a tool to assess not only which components of the model affect the projections the most but also the confidence that should be placed on those projections. In addition, if the sensitivity analysis is extended to include an evaluation of changes in advective flow and pollutant loading, then the effectiveness of alternative management proposals can be evaluated critically.

The committee also agrees that because of the large random component inherent in environmental data, application of stochastic modeling techniques to the sensitivity analysis of model projections should be encouraged. At present, Monte Carlo simulations appear to be the most straightforward technique for stochastic modeling.

Issue 6: Models as Projection Tools

Since the model to be used for projection analysis ideally should be developed on the basis of intimate knowledge of the drainage basin, its problems, and potential management strategies, the modeler should be able to anticipate the needs of the decision maker and thereby avoid having to push the model beyond its intended limits. Hence, the modeler should be able to make projections within these limits with considerable confidence and reliability given sufficient understanding of the following:

1. Parameter adjustments to projection conditions - flow, temperature, boundary conditions, sources and sinks of oxygen, etc. - with as many parameters explicitly related to causative mechanisms (e.g. reaeration rate to hydraulic properties) in order to eliminate subjectivity in their selection.

2. Variability factors as they influence the allowances that must be made in comparing model results to standards.

3. Risk involved in the decisions which are to be made and the required sensitivity analysis on the model projections.

4. Frequency of compliance with standards and related questions.

The degree to which each of these four issues has to be incorporated into design of the projection analysis program varies of course from site to site. However, the analyst must always be mindful that the goodness of the verification is a key measure in determining how conservative the projection analysis should be.

In conclusion, the committee agrees that a DO/TEMP model based on good synoptic type data and on rigorous calibration and verification procedures is a valuable tool in the evaluation of alternatives for the decision maker.

RECOMMENDATIONS

of the

Dissolved Oxygen/Temperature Committee

A number of recommendations emerge naturally from this assessment of the state-of-the-art of DO/TEMP modeling.

1. The committee unanimously agrees that development, calibration, and verification of a reliable specific case model depends on an intensive synoptic type data acquisition program. The design of such a program in its essential elements is presented in the discussion of Issue 2: Data Base. It is strongly urged that such programs be encouraged and supported at all levels of decision making.

2. It was further agreed that while water quality monitoring-type data may serve a useful purpose in regulatory and compliance practice it should not be used in modeling practice because this type of data only measures the in-stream response to unknown source loadings.

3. It was further agreed that long hydrological and meteorological data acquisition programs should be not only continued but expanded in coverage since all DO/TEMP projection analyses are inescapably tied to probability of occurrence of these natural phenomena.

4. It was further agreed that kinetic detail in the formulation of specific case DO/TEMP models should be limited to that required to adequately reproduce the primary state variable interactions.

5. It was further agreed that the practice of using inappropriate data, of using reaction rates gleaned from the literature without proper in-situ validation, and of using the same data for "verification" as was used for calibration is not acceptable and is to be strongly discouraged.

6. It was further agreed that a better phenomenological understanding of reaeration leading to a better predictive equation is urgently needed.

7. It was further agreed that follow-up studies should be conducted on the watercourse after a course of action based on model projections has been implemented.

8. The committee agrees furthermore that statistical analysis can be a valuable tool for quantifying the "goodness of fit" between the observed and predicted profiles and that use of verification "scores" should be encouraged but not promulgated.

9. Studies should be instituted to incorporate verification testing techniques into existing computer programs including appropriate mass balance checks.

10. Although it is impossible to develop a universal water quality model to suit all needs, efforts should be made to make the format of modeling output as uniform as possible. This would enhance the transfer of modeling results and also make modeling more acceptable to decision makers. In addition, computer graphics techniques should be encouraged in relation to the presentation of modeling results.

11. Finally, it was agreed that modeling should not be marketed as a quick, easy, or magical way of providing wholesale answers to water quality problems.

STATE-OF-THE-ART REPORT

of the

Bacteria/Virus Committee

John L. Mancini - Chairman

Members

Raymond Canale	John A. Harris
G. Wolfgang Fühs	Alan I. Mytelka

Issue 1: Role of Models in Decision Making

The state of the art for modeling virus distributions cannot support decision making.

Decision makers have a healthy skepticism of models. On the other hand, models have provided a rational basis for decision making when properly applied and these proper applications should be supported. In addition, a more open communication of management needs and model capabilities and limitations should be encouraged.

Models which calculate the distribution of coliform bacteria can be used for planning and design decisions in streams, estuaries, oceans and lakes. Some reservations exist, as expressed by both managers and engineers, but these can be overcome in many instances by inclusion of appropriate safety factors and/or staged construction of facilities.

Issue 2: Data Base

Data available from data banks (STORET, surveillance networks) are generally inadequate as input for models, and special data gathering efforts are needed for each study. Intermittent sources (storm sewers, combined sewer overflows) are to be sampled in the study area, but data gathered in similar studies on a comparable area can be used with confirmation. The emphasis in sampling should be on the study of storm events of different types and durations (as characterized by hydrographs) and periods of dry weather between storms (a minimum of 3 to 6 storms per outfall are needed). As a minimum, both the mean and variance of the concentration of indicator bacteria are to be determined for each event. Some committee members believe that land use patterns are useful for the selection of representative sampling sites.

Data collection to define rates of die-off of indicator bacteria, in the opinion of most committee members, should be continued with special attention to variations in die-off rates in different types of receiving waters.

For pathogens loss of viability is insufficiently known, and factors such as adsorption and sedimentation may have to be considered.

Coliform and pathogen densities cannot be determined in the presence of solid raw sewage matter.

Issue 3: Time and Space Scales; Kinetic Detail; Cost Effectiveness

Typical temporal and spatial scales are relatively short, but are specific to the questions asked of the model and the complexity of the system being analyzed. Evaluation of the transport phenomena and the rates of reactions will define these scales. The bacterial kinetics can be extrapolated from previous studies, but require substantiation by short-term field tests to ensure proper orders of reaction.

Basic planning decisions and the majority of detailed design and operational actions can be accommodated by a steady state model. However, as the system under evaluation becomes more complex, especially through influences of transport, dynamic simulation procedures need to be used.

Although the software for bacterial modeling is relatively simple, incorporation of internal checks, e.g. mass balance summaries, should be used. Emphasis needs to be placed in the integration of the physical influences on the bacterial kinetics.

A "standard numerical solution" for simple situations would be helpful as would standard examples for specific software.

Issue 4: Parameter Estimation

The kinetic coefficients for models of indicator bacteria are best obtained on a site specific basis using a three step procedure. First, a good field sampling program is conducted which is compatible with the model framework and has simultaneous measurements of all the important variables and processes such as the water quality response, loadings, flow patterns and dispersion. These results are used in conjunction with the model and a trial-and-error procedure to estimate the bacterial die-away rate. Next, this rate should be compared with estimates obtained from in situ bottle or bag studies where bacterial concentration changes are followed over time in a uniform mixture of the wastewater and the receiving water. Finally, estimates of die-away rate should be compared to literature values. For the case of indicator bacteria, die-away rates are relatively well-known functions of temperature and salinity. Thus, because the kinetic framework for indicator bacteria is normally quite simple, relatively straight-forward and standard procedures can be used to estimate the kinetic coefficients.

Issue 5: Measures of Verification

Present procedures in verifying models are to use caution, review similar situations, and to apply engineering and other practical experience in judging model predictions.

The overall sentiment is that a set of statistical techniques should be promulgated. The range of opinion varied from strong support to strong opposition. In support of promulgation is the proposition that models and their use is a fact of life, even though models are sometimes being misused and the model predictions are often being given more weight in decision making than warranted. Being able to quantitatively describe their credibility should improve understanding of applicability. The strong dissent to promulgating quantitative statistical techniques centers on the concern that statistical justification is too easily fabricated so as to impress decision makers and reinforce their acceptance of a level of credibility of models that is not justified.

Issue 6: Use of Models as Projection Tools

The committee generally felt that in their present state models of indicator bacteria could be used in the projection mode, although one committee member was skeptical of their credibility. Proper application of basic conservation of mass equations, coupled with a knowledge of the literature of bacterial kinetics, would be appropriate for many planning problems. The committee had differing views on the method of providing for recognized uncertainities in the accuracy of results. Some felt that monitoring of control sites would best minimize uncertainties while others felt that staging of construction and/or providing sufficient factors of safety would be more appropriate.

Summary

Bacterial modeling is being effectively applied to provide input for broad management decisions. Increases in difficulty are experienced considering detailed design and operational decisions when bacterial models are applied to complex receiving water systems. These difficulties result primarily from lack of information on the transport phenomena and lack of proper verification techniques to validate the model structure.

Models for indicator bacteria can be used with a relatively high degree of confidence for many planning and design problems when the results are employed in close conjunction with professional engineering judgment and intensive calibration and verification field sampling programs.

RECOMMENDATIONS

of the

Bacteria/Virus Committee

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1. Committee agreement was obtained, in principle, on the importance of evaluating health risks associated with bacterial bathing and shellfishing standards. The Committee had divergent views as to when efforts should be devoted to this area. One approach suggested steady investments in this area over time whereas an alternate view was that funding should be contingent upon identification of some benefits, i.e., cost reduction, health improvements, et al.

2. Work on relative die-away rates for pathogens and viruses as compared to the indicator bacteria should be supported.

3. Methods of estimating wastewater inputs which efficiently meet requirements are needed. For intermittent inputs, these requirements are:

    - Accurate measures of the number of organisms discharged on an event basis.

    - Variance in concentration of organisms in the discharge in individual events and over a large number of events.

4. Virus evaluations would be useful particularly since current thinking appears to be that health effects at beaches and in shellfish are primarily associated with viral infections. In this regard, improved measurement techniques are required and quantification of virus counts in wastewater discharges are mandatory. Work on determining viral die-away rates is recommended as well as development of dose-response relations. Finally, methods should be employed to track viruses ("hot" particles) to insure that significant processes are being accounted for (affinity for solids, etc.).

5. Other phenomena which may be present and significant should be more fully defined such as:

- After growth
- Reduced rates of mortality at low bacterial concentrations.
- Effects of salinity on die-off rates in subsurface waste fields in marine environments.

6. The level of complexity needed for the definition of transport fields is, to some extent, problem and site specific. Therefore a fruitful area of research would be associated with development of transport field assessment methods of varying levels of complexity which could be calibrated and/or verified independently of the bacterial analysis.

7. There is agreement that a need exists to evaluate modeling results. There are two aspects which should be considered:

    - How good is the model?
    - What input can the model make to the decision making process?

    The committee encourages further thoughtful R & D efforts to develop technology in these areas.

STATE-OF-THE-ART REPORT

of the

Eutrophication Committee

Dominic M. DiToro - Chairman

Members

Robert Ambrose
Michael A. Bellanca
Carl W. Chen
John M. Higgins
Tavit Najarian
Donald Scavia
Kent W. Thornton
G. Kenneth Young

Issue 1: Role of Models in Decision Making

The committee feels that decision makers often expect too much from models and that qualified results given to the manager are more useful than no result at all. Given all other factors that enter into a water resource management decision, it may not be worthwhile to delay decisions for a finally verified model.

Issue 2: Data Base

The data base available is generally inadequate with infrequent sampling of too few variables. Data gathering is sporadic rather than synoptic and is usually not coordinated with a modeling study. It is to be noted that appropriate sampling intervals on an annual cycle are not uniform and are strongly dependent on the particular water body being studied.

There is a paucity of rate measurements as well as benthic-sediment information. STORET should be continued with an emphasis on quality control of the input data. A higher priority should be given to developing a biological data management system which includes a taxonomic hierarchy. Special data bases in the system are quite good such as for the Great Lakes. The data base needs additional nutrient information especially at low concentrations as well as better chlorophyll and biomass data. At present there is a functional problem with soluble reactive phosphate and procedures for filtered nutrients should be defined, or refined, to incorporate nutrient measurements that indicate functionally available forms for uptake.

There are generally deficiencies in the point source data with a lack of sample replication. Non-point source data are also required for both storm event and base flow conditions.

Issue 3: Time and Space Scales; Kinetic Detail; Cost Effectiveness

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There are no universally accepted criteria for selection of an appropriate modeling framework. Factors considered important by committee members include: financial resources available, complexity of the system, the problem and questions to be addressed, the projected time horizon, available technology and the ability of the selected framework to analyze alternatives.

The committee feels that there is a clear and present danger in the validation (or lack thereof) of computer software in the eutrophication area. Due to the complexity of the interacting systems, code must be thoroughly checked for programming errors and numerical errors. The analyst should utilize known mass conservation laws, check results against available analytical solutions and consult with other users to elicit any known deficiencies. Test cases for code and standard solutions for judging the adequacy of the software should be provided.

Issue 4: Parameter Estimation

Parameters are generally selected by choosing values within reasonable ranges, by a best fit procedure and by exercising judgment. Values should be selected for the appropriate type of water body and care must be employed not to mix marine, brackish and freshwater parameters. Some assistance is available in recently published rate manuals but this is no substitute for experience.

Credibility of selected parameters is judged by comparison to known ranges of the values with careful analysis of any extreme values. In addition, sensitivity analysis is used to determine if the model results are hypersensitive to slight perturbations in a parameter. Monte Carlo simulations of kinetic constants are helpful in assessing system sensitivity to the parameters. Finally parameters are judged credible if kinetic fluxes are reasonable, i.e., if the fluxes calculated with the parameters compare well to independent measurements such as primary productivity.

Automated methods presently exist which minimize the differences between observations and calculated results by varying parameters. The committee urges that these methods be used within specified bounds and that judgment be used to avoid simple curve fitting. Any statistical methods developed to aid in parameter estimation ought to estimate both total system and parameter errors and be able to identify any systematic errors or biases.

Issue 5: Measures of Verification

In calibrating a model reasonable coefficients are selected such that measured data compare well with model output and calculated fluxes are reasonable when compared with independently determined fluxes. In this calibration phase also, care is taken to search the output for any non-explainable computational results. During the verification phase, data withheld during calibration (split data set) is used commonly to test the validity of the model. In addition, data sets with statistically different characteristics are used together with their associated different input conditions. It is suggested that verification - in the sense of achieving truth - is too strong a goal. On the other hand, verification - in the sense of "acceptance testing" - is strongly encouraged by the committee.

Credibility of the model is established through: internal consistency; minimizing empirical formulations without observational support; applicability of the model to similar situations; demonstrated predictive ability; absence of any counter-intuitive non-explainable results and use of reasonable assumptions for the inclusion or exclusion of normally significant mechanisms.

In establishing model credibility, the use of statistical techniques should be recommended (not promulgated). Goodness of fit tests should be employed, with the number of degrees of freedom minimized (e.g. 100 parameters for 80 data points). Analysis of residuals should be employed to test for lack of bias, randomness and normality - the latter if assumed in the statistical method. Least squares techniques should be used on single decision variables and weighted least squares on multiple decision variables. In assessing goodness of fit, penalties should be assigned more strongly to either underestimations or overestimations depending on the variable being tested (e.g. one sided loss function for dissolved oxygen). It may be noted that some data sets are not of high enough quality or are of too small a sample for meaningful statistics.

Issue 6: Use of Models as Projection Tools

In selecting projection conditions, there are no well defined criteria to assist the analyst. It is clear that as many potentially critical conditions should be examined, as is consistent with the resources available.

The committee was divided in their assessment of the ability of eutrophication models to predict incremental water quality changes in the future, with the nine members characterizing it as follows: good (3), fair (5), poor (1). Likewise, the credibility of model results for presently non-existent systems (e.g. new reservoirs) were adjudged to be: good (1), fair (5), poor (1), no opinion - case by case evaluation (2).

Summary Question

Overall, the committee judged the present state of the art of verification of eutrophication models to be either fair (2 members) or poor (6 members) and the credibility of these models to be generally good to fair (good-3, fair-4, poor-1).

RECOMMENDATIONS

# of the

Eutrophication Committee

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1. Credibility of models can be improved by:

   a) early communication with decision makers to clarify water uses, problem areas and project requirements
   b) more emphasis on data collection and less on analysis
   c) quantification of "how good" and "how bad" the model predictions are
   d) improved methods for visually displaying modeling results (e.g., automated computer graphics)
   e) complete model documentation at all levels (computation can be reproduced from the report only)
   f) complete candidness on modeling with no "overselling" of its capabilities
   g) implementation of post-auditing procedures

2. Traveling "road shows" are recommended for explanation of model capabilities and applications to decision makers.

3. In data gathering, new technology should be employed, such as remote sensing of chlorophyll and turbidity (LANDSAT - Nimbus G).

4. For wastewater inputs, it is recommended that continuous sources be monitored for nutrients using flow composited daily samples. After a preliminary study to determine its importance, non-point source information should be gathered with at least two data sets, one for calibration and one for verification. The non-point data should be coordinated with appropriate land uses and the total non-point discharge to a water body estimated from its total drainage area.

5. Field scale experiments should be conducted with major perturbations to the system (e.g. addition of large quantities of nitrogen or phosphorus), which are closely coupled with calibration and prediction computations. During these field studies a sufficient number of measurements of fluxes and state variables would be made.

6. It is recommended that a number of "National Benchmark Lakes" be established with full data sets, against which all models might be tested ("standard solution").

7. Water quality standards which relate eutrophication variables to water use and impact should be developed. Dissolved oxygen is an important secondary variable that should be considered here.

8. It is recommended that a simple model calculation (e.g. mass balance) always be used whether or not a complex calculation is attempted. From a consultant's point of view, an answer must be obtained within the allocated time and money and complex model calculations often are not guaranteed. It is also not clear whether the uncertainities in the results are smaller or larger when one compares results from simple and more complex models.

9. Resources should be allocated for post-auditing of water bodies after changes in the system are implemented. Staged construction is recommended where uncertainities exist, with a reanalysis of new data prior to continued construction.

10. Increased use of computer graphics should be made for display of model output.

11. Computer based eutrophication models should be used only by professionals in the field.

STATE-OF-THE-ART REPORT

of the

Hazardous Substances Committee

Tudor T. Davies - Chairman

Members

David Alexander	Yasuo Onishi
Thomas W. Gallagher	William L. Richardson
Richard C. Graham	Phillip L. Taylor
John P. Lawler	James Tofflemire
W. Brock Neely	

Issue 1. Role of Models in Decision Making

The committee felt that modeling in the hazardous substance area often is not a factor that comes into play in decision making. On the other hand, it was also noted that managers often readily embrace modeling results that can be best characterized as "non defensible number generation." Concern was expressed with respect to a proper balance between the role of health effects and the role of good modeling. The committee viewed modeling as one of the many tools that should be used carefully in the decision making process, examples of which process are illustrated in the two figures that follow.

Issue 2: Data Base

The committee felt that data available in the hazardous substance area was totally inadequate and, in many ways, unreliable (e.g. the method of analysis sometimes in error). In the absence of good predictions of cohesive sediment migration, adequate sediment procedures are needed. It was felt that input load data generally provided highly variable estimates and that the receiving water quality data base was meager and often in error. There is a paucity of information on model parameters of hazardous substances which depend on adsorption/desorption, partition coefficients and cohesion coefficients of fine sediment.

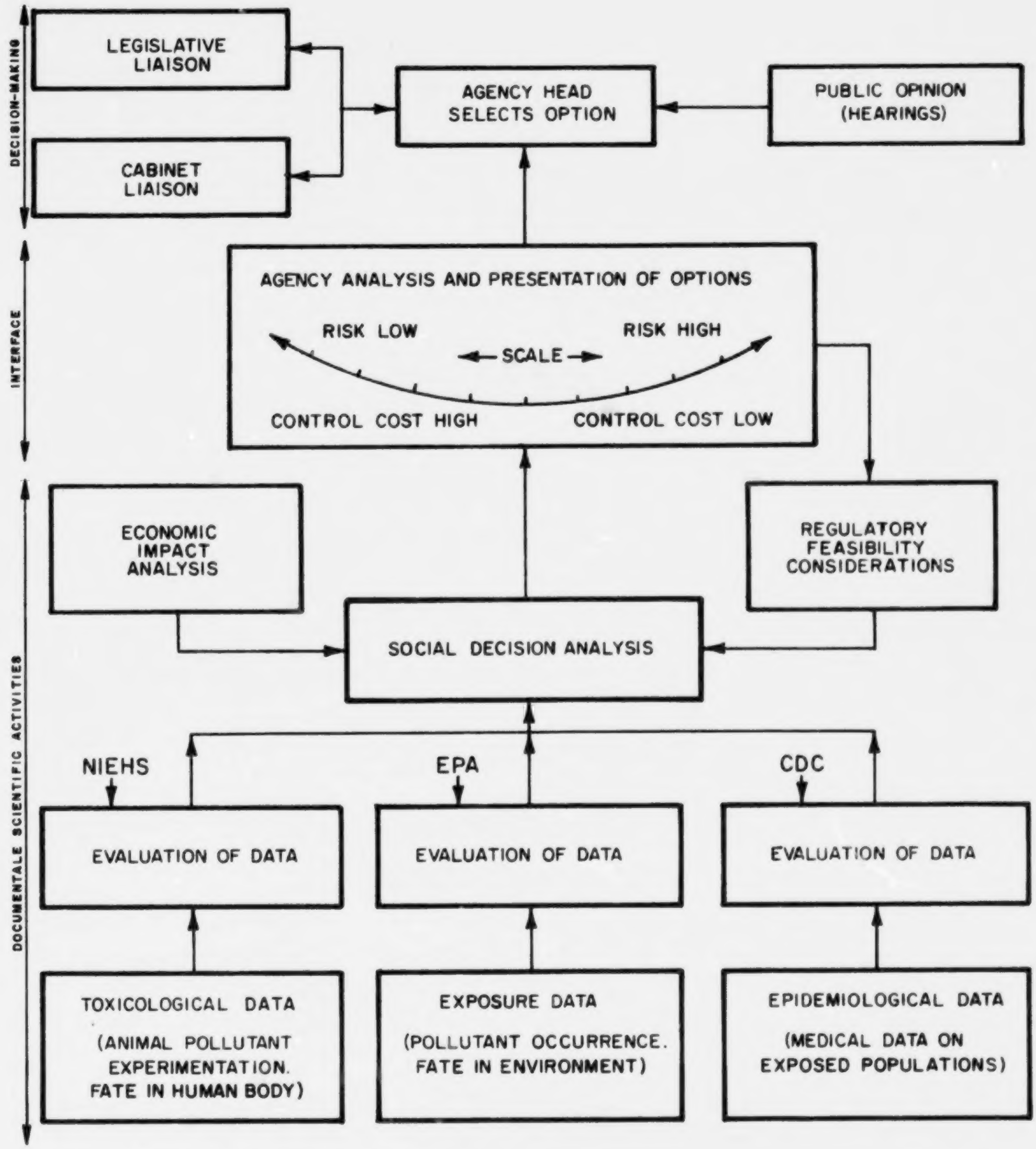
DECISION-MAKING
LEGISLATIVE LIAISON
AGENCY HEAD SELECTS OPTION
PUBLIC OPINION (HEARINGS)
CABINET LIAISON
INTERFACE
AGENCY ANALYSIS AND PRESENTATION OF OPTIONS
RISK LOW
RISK HIGH
SCALE
CONTROL COST HIGH
CONTROL COST LOW
DOCUMENTALE SCIENTIFIC ACTIVITIES
ECONOMIC IMPACT ANALYSIS
REGULATORY FEASIBILITY CONSIDERATIONS
SOCIAL DECISION ANALYSIS
NIEHS
EPA
CDC
EVALUATION OF DATA
EVALUATION OF DATA
EVALUATION OF DATA
TOXICOLOGICAL DATA
(ANIMAL POLLUTANT EXPERIMENTATION. FATE IN HUMAN BODY)
EXPOSURE DATA
(POLLUTANT OCCURRENCE. FATE IN ENVIRONMENT)
EPIDEMIOLOGICAL DATA
(MEDICAL DATA ON EXPOSED POPULATIONS)

FIGURE I. DECISION-MAKING IN THE REGULATION OF TOXIC SUBSTANCES

e.g., U.S. GOVT.

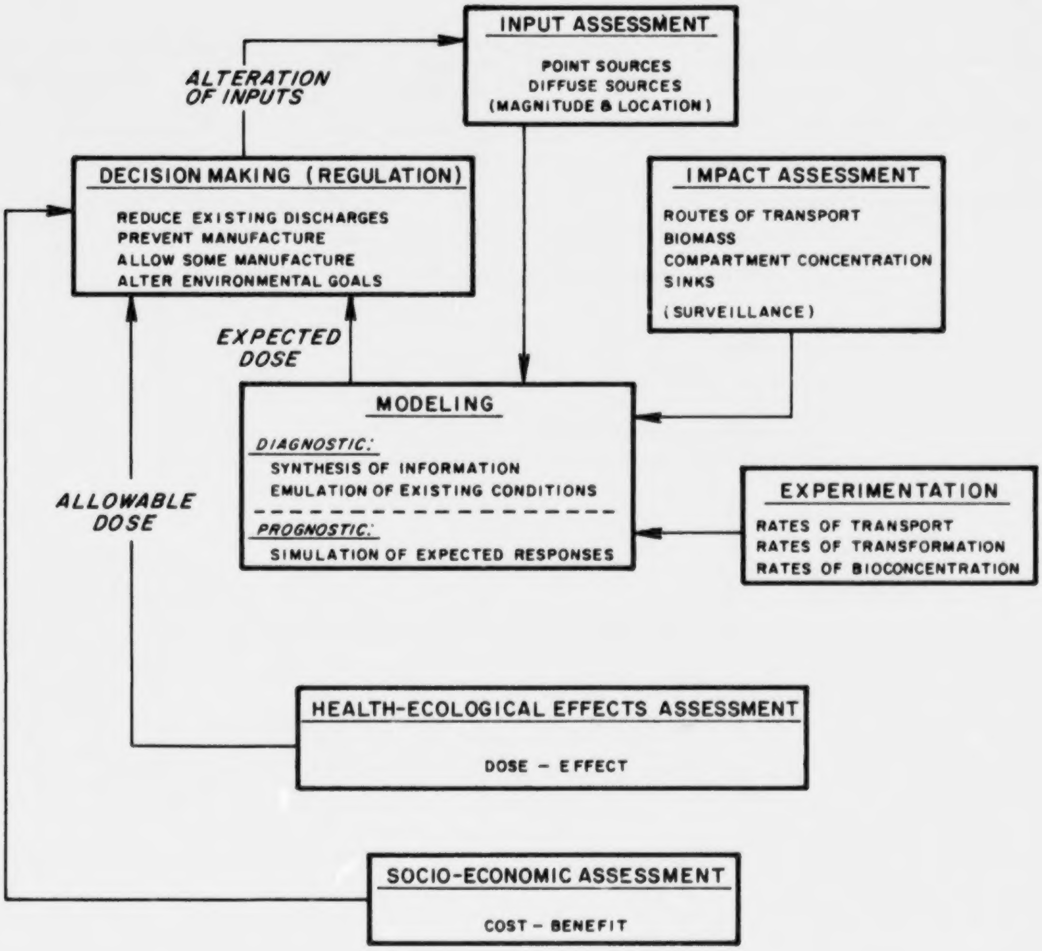
INPUT ASSESSMENT
POINT SOURCES
DIFFUSE SOURCES
(MAGNITUDE & LOCATION)
ALTERATION OF INPUTS
DECISION MAKING (REGULATION)
REDUCE EXISTING DISCHARGES
PREVENT MANUFACTURE
ALLOW SOME MANUFACTURE
ALTER ENVIRONMENTAL GOALS
IMPACT ASSESSMENT
ROUTES OF TRANSPORT
BIOMASS
COMPARTMENT CONCENTRATION
SINKS
(SURVEILLANCE)
EXPECTED DOSE
MODELING
DIAGNOSTIC:
SYNTHESIS OF INFORMATION
EMULATION OF EXISTING CONDITIONS
PROGNOSTIC:
SIMULATION OF EXPECTED RESPONSES
ALLOWABLE DOSE
EXPERIMENTATION
RATES OF TRANSPORT
RATES OF TRANSFORMATION
RATES OF BIOCONCENTRATION
HEALTH-ECOLOGICAL EFFECTS ASSESSMENT
DOSE – EFFECT
SOCIO-ECONOMIC ASSESSMENT
COST – BENEFIT

FIGURE 2. ENVIRONMENTAL MODELING MANAGEMENT PROCESS

It was suggested that workers in this area need to take advantage of the available radionuclide data base.

Issue 3: Time and Space Scales; Kinetic Detail; Cost Effectiveness

Selection of a modeling framework is quite dependent on the problem being addressed and must include considerations of the impacts on both man and the biota. The spatial scale of the model would extend over that distance within which the toxicant would have an impact on man and the biota and this would be a function of the operative mechanisms. Temporal scales would vary from days to several years, depending on the specific kinetics and transport, the seasonal effects (wet vs. dry weather) and the type of release (instantaneous vs. continuous release). Major kinetic mechanisms that are to be examined in the modeling of hazardous substances include sediment interactions with the toxicants, chemical changes and bioaccumulation.

The committee felt that a standard validation procedure should be used to check computer software and that, to the extent possible, analytical solutions should be made available. It was noted that computations should be performed in consistent units such that mass balances could be performed. Second party review was also recommended for validation as well as use of another computer code which had been applied to similar problems.

Issue 4: Parameter Estimation

In estimating model parameters, the committee felt that measurements for chemical and physical mechanisms should be performed first. After field measurements for transport parameters are accomplished, laboratory measurements of the physical and chemical properties of the hazardous substance are made, related to the various variables upon which a specific parameter depends, and translated to field conditions. Laboratory rates of hydrolysis, oxidation, evaporation and photolysis are related directly to field conditions, whereas sorption/desorption kinetics are dependent on the nature, size distribution and type of solids in the natural system.

Translation of laboratory data on biological parameters to field conditions is an order of magnitude more difficult than for the physical/chemical rates and workers should expect to perform field measurements. Laboratory measurements, however, are useful in partitioning uptake pathways.

Credibility of the selected parameters is established through sensitivity analysis, by comparson with scientifically defensible ranges of values of the parameters and by selection of parameters using means independent of the model.

Issue 5: Measures of Verification

In the calibration and verification of models, the committee reported that comparison of model output to observed data is a basic mandatory procedure together with checks on the conservation of the total mass. Credibility of the model is judged by examining whether recognized mechanisms and parameters are used, the degree of reliance on observed data to establish parameter estimates and the history of success of the model or similar models. In addition, the relative confidence in each of the model elements, via-a-vis both mechanisms and parameters, is used to judge overall model credibility.

The committee felt that a set of statistical techniques should be used to quantify model credibility with neither blind rejection of the model, if the statistical criteria are not met, nor blind acceptance of the model if the criteria are met.

Issue 6: Use of Models as Projection Tools

The selection of the projection conditions for modeling of hazardous substances incorporates the following considerations: problem definition, acceptable level and frequency of risk, the level of "insurance" a client is willing to pay for, chronic vs. short-term effects and existing vs. proposed chemicals. It was noted that these substances-unlike others such as dissolved oxygen, temperature, salt, etc.-have been introduced by man and a different type of criteria than used for other substances may be appropriate and should be developed. It was also noted that tools for comparable evaluations of the impacts of various hazardous substances or on the effectiveness of various control strategies should be available.

The committee felt that models of hazardous substances could describe incremental water quality changes under future design conditions, at least to the level of an overall macroscopic mass balance.

With respect to model credibility for systems where data do not exist (physically non-existent system), the committee felt that adequate results were possible if models included recognized mechanisms and parameter values - whose relative confidence were known-and the models had a history of success being applied to the specific, or similar, problems.

RECOMMENDATIONS

# of the

Hazardous Substances Committee

The Committee recommends that another workshop be reconvened with plenary lectures given by USEPA personnel on the state of their mass balance models for hazardous substances. The workshop should be directed toward recommendations on how to improve the macroscopic scale models, i.e. make them more microscopic. This may entail three of four pilot studies where sufficient data would be obtained on a few chemicals - including radionuclide tracers - so that micro-scale models can be calibrated, verified and post-audited.

HOW A PROGRAM MANAGER USES WATER QUALITY MODELS

By

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The program manager is one link in the decision-making process. He may only make recommendations to a funding entity, but his evaluation of alternatives and selection of a recommended action have a strong influence in the decision-making process. He can use water quality models for two purposes: 1) as a planning tool to compare alternatives; and 2) as evidence in support of recommendations. The same modeling information may be used for both purposes. The program manager's understanding of the modeling information will determine how well he is able to support his recommendation when questioned.

In planning, models are only one source of information when comparing alternatives. There may be projections of population or of water resource development. There will be calculations of costs and benefits, and an economic analysis which may include predicted rates of inflation. All projections are uncertain to some degree. Population projections may err numerically or in distribution patterns. Cost estimates often have a contingency factor of 25 or 30 percent. Benefits may err with respect to both production and prices. But estimates must be made, then detailed calculations are performed on these estimates.

Seldom is a water quality model the one key element in the planning process. The relative worth of all the inputs must be considered. If the water quality model results are considered 75 percent reliable, and cost estimates and other environmental effects have a 90 percent reliability, the latter would be given more weight.

When modeling results are used to support the program manager's recommendations, he would like very positive and unequivocal information, but he knows there will be qualifications. There must be communication between the program manager and the modelers. The modelers should not hesitate to inform the program manager of any shortcomings they perceive in the model or concerns that they may have. He does not want to learn of these shortcomings from someone else during a public hearing.

The program manager will feel more confident with his recommendations if a sensitivity analysis of the model results can be done for him. When he knows that the variation of a parameter over a wide range results in a small variation in model results, he will feel more comfortable.

In summary, the program manager wants as much information as possible that is relevant to a recommendation. The modeler should communicate extensively with the program manager and not assume that the program manager is well versed on modeling. It is the modeler's responsibility to inform him as thoroughly as possible.

WATER QUALITY MODELS FOR BACTERIA AND VIRUSES

By

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Introduction

This discussion concerns the modeling of bacteria and viruses in the context of the six "issues" raised by the organizers. The emphasis will be on modeling of indicator bacteria because we have had limited experience (especially of a practical nature in actual field situations) with virus problems.

Issue #1 - Role of Models in Decision Making

Unfortunately, far too often administrators do not use model output to arrive at rational wastewater management decisions. Even more tragic is the fact that frequently these same administrators financially support the development of models and then fail to use them. These kinds of experiences errode the credibility of the only quantitative technology which can respond to environmental impact problems in a rational fashion. To avoid these difficulties it is important that modelers and administrators cooperate during the initial phases of a project and jointly define the users of the model in terms of water quality issues. This should lead to proper model design with regard to time scales, space scales, and kinetic and hydraulic complexity. Unfortunately, in many cases the water quality issues are forced to fit the framework of readily available "shelf" models rather than the other way around as suggested above. As a result the models are either too simple to address the real problems, or worse, too complex to interpret.

A second major deterrent to effective use of models by administrators concerns the degree of confidence both modeler and administrator have in the ability of the model to represent the real system. Model design should respond to the individual characteristics of each lake or river in the simplest possible manner and avoid unnecessary mathematical complexity. The use of general "off the shelf" models should be avoided. The resultant models should then be carefully calibrated and verified prior to application.

Issue #2 - Data Base

A critical factor related to model use by administrators concerns the availability of adequate data for model calibration and verification. Station locations and sampling frequency should be compatible with the time and space scales of the model, which is in turn related to model use. It is necessary that the system response water quality be measured during periods when all pollutant sources are known by simultaneous measurement. Sampling stations should be located to simplify estimation of model coefficients during calibration. It is also important to coordinate measurement of other variables during sampling such as advective flow patterns, dispersion coefficients, temperature and boundary concentrations.

Normally routine monitoring data are of little value for calibration or verification of models for indicator bacteria. This is the case because monitoring programs do not normally include measurement of all of the important variables and have deficiencies with regard to both sampling frequency and location. Thus, the value of monitoring data is normally limited to surveillance purposes. Modeling programs which must rely on existing monitoring data are normally doomed to failure because of these inherent limitations. When these restrictions are imposed it is difficult to properly design, calibrate, or verify models. These are the reasons models are not used by administrators.

Issue #3 - Model Detail

Probably the most important principle of model design is that the framework of the model should be the simplest possible that permits description and quantification of the important phenomena operating in the lake or river. Thus linear die-away kinetics are used unless nonlinear processes can be shown to be important to the problem solution, despite the fact that real systems involving indicator bacteria are nonlinear. It is advisable to use simple hydraulic models when complex ones can be avoided. For example, it is poor engineering practice to construct models for instantaneous tidal velocity if only long-term or time-averaged spatial concentration profiles are required for problem solution in terms of the water quality issues. Interactions with administrators are necessary to insure proper model design. Complex questions for some problems such as temporary pollution levels associated with combined sewer overflows during wet weather events may require construction of complex time variable models, but simple models should be designed if possible.

Issue #4 - Parameter Estimation

The kinetic coefficients for models of indicator bacteria are best obtained on a site specific basis using a three step procedure. First, a good intensive field sampling program is conducted which is compatible with the model framework and has simultaneous measurements of all the important variables and processes such as the water quality response, loadings, flow patterns, and dispersions. These results can be used in conjunction with the model and a trial-and-error procedure to estimate the bacterial die-away rate. Next this rate should be compared with estimates obtained from bottle test studies. In this text bacterial concentration changes are followed over time in a uniform mixture of the wastewater and the receiving water. Finally, estimates of die-away rate should be compared to literature values. For the case of indicator bacteria, kinetic die-away rates are relatively well-known functions of temperature and salinity. Figures 1 and 2 show the results of two independent data summaries which define first-order bacterial die-away rates. The results for freshwater are relatively similar despite the different sources of data. Thus, because the kinetic framework for indicator bacteria is normally quite simple, relatively straight-forward and standard procedures can be used to estimate the kinetic coefficients.

Issue #5 - Verification

It is necessary to verify models for indicator bacteria because during calibration laboratory die-away coefficients are adjusted to accomodate settling and other phenomena which may not occur in the bottle test. Thus, it is essential that the model output be checked against field data for at least one independent set of conditions. It is advisable that more than one independent survey be used if possible because measurement techniques for indicator bacteria are not very precise. The goodness of fit of the model compared to field data may be evaluated using recent statistical methodologies proposed by Thomann (1979). In addition it is advisable to perform sensitivity calculations to determine how the model output varies as a function of changes in model coefficients and forcing functions. It is important that the modeler have accurate estimates for the most sensitive variables.

Issue #6 - Use of Models as Projection Tools

Mathematical models for indicator bacteria should ideally be used to evaluate the marginal costs and benefits associated with incremental changes in water quality. As an example Figure 3 shows a plot of fecal coliform loading vs. the resultant fecal coliform concentration as calculated by a model in critical regions of Onondaga Lake. Cost of treatment can be related to loading for various degrees of control of combined sewer over-

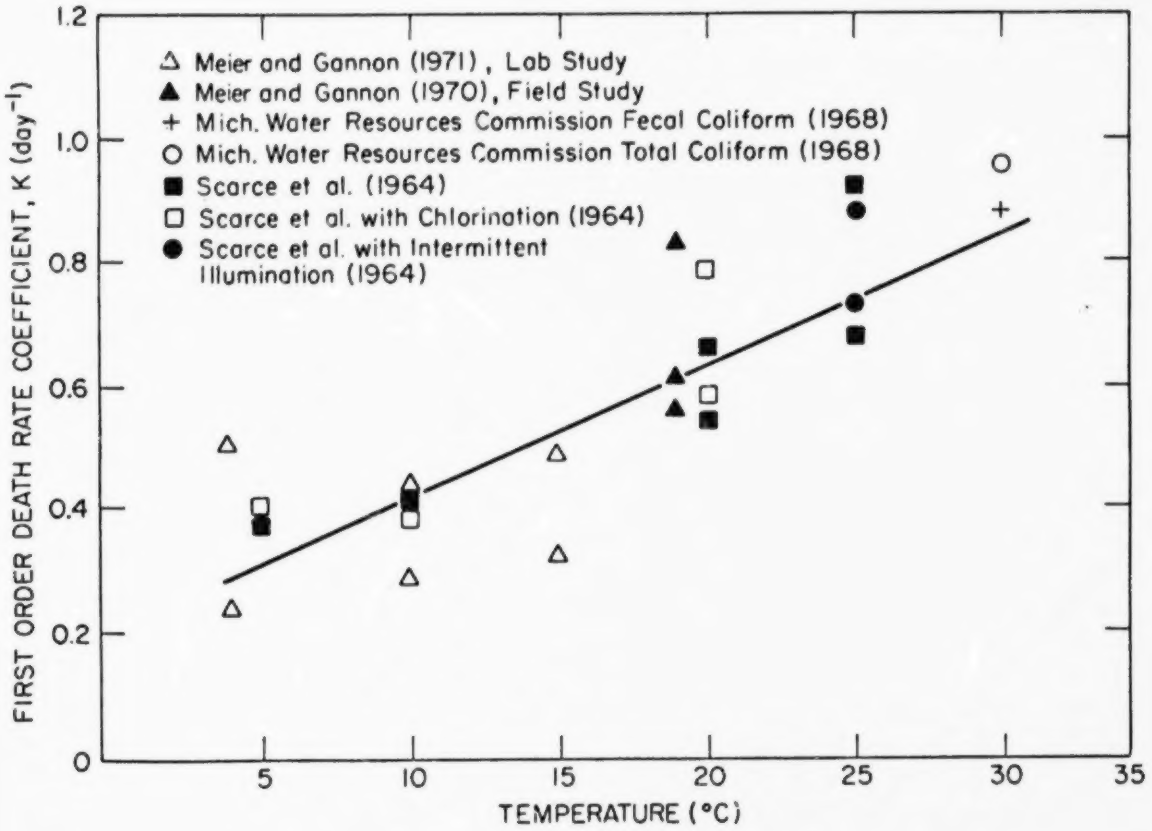

FIGURE I. BACTERIA DIE-AWAY RATE AS A FUNCTION OF TEMPERATURE

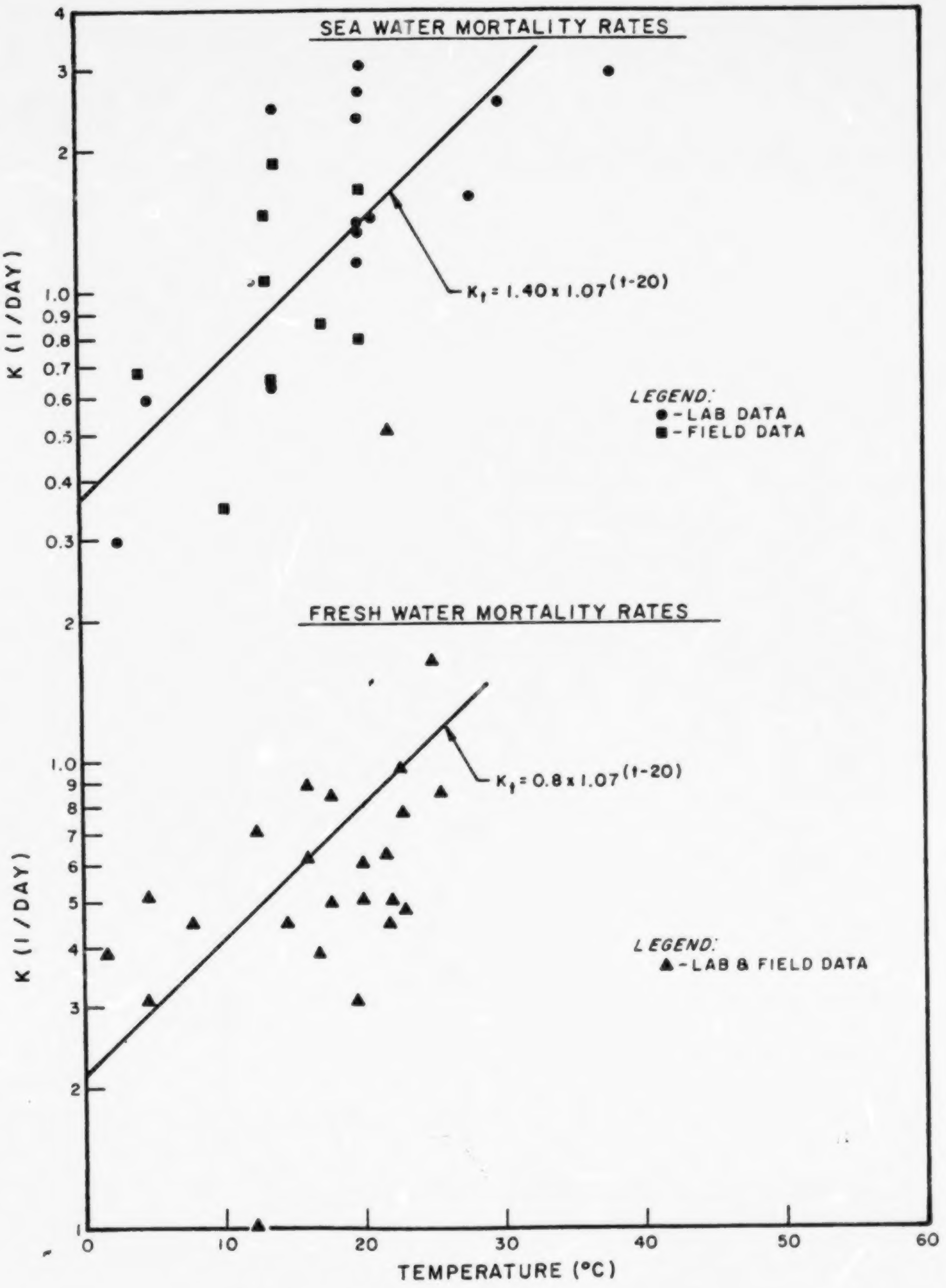

FIGURE 2. BACTERIA DIE-AWAY AS A FUNCTION OF TEMPERATURE

(MANCINNI, 1978)

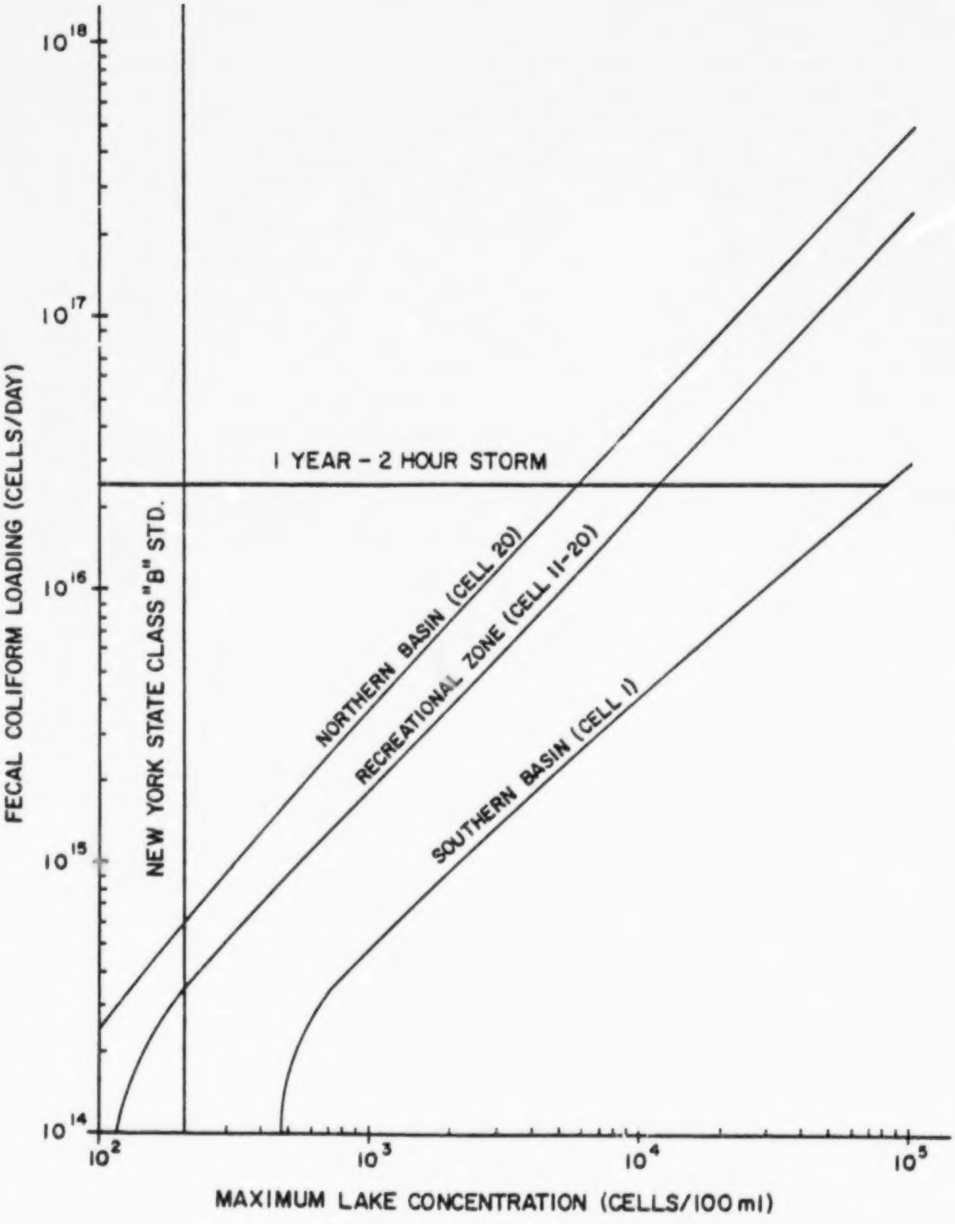

FIGURE 3. FECAL COLIFORM LOAD VS. MODEL CALCULATED MAXIMUM LAKE CONCENTRATION DURING WET WEATHER CONDITIONS IN ONONDAGA LAKE, NEW YORK

flow. Although similar relationships have been developed between loading and response for many other projects, an important question concerns the accuracy of such calculations. Errors are introduced into the projections because the model coefficients, forcing functions, and initial conditions are not known perfectly. These types of errors occur even if the model structure and mechanisms are assumed to be perfect (which is never the case). Normally, these questions are addressed by sensitivity analyses of the results to design conditions. A better approach to this question would be to perform Monte-Carlo simulations where all the uncertain values are varied in a random fashion over the full range of uncertainity. Unfortunately this is a costly procedure which is rarely used in engineering practice. Research now being conducted at the University of Michigan is examining the applicability of Kalman filtering techniques for calculating directly the probable error associated with model projections as a function of the error in the model coefficients and forcing functions. This capability will in turn help determine in a quantitative manner the amount of data necessary to verify model frameworks, coefficients and forcing functions. It is hoped that this type of systematic approach to a problem which has been formally addressed mainly on an intuitive or judgment basis will ultimately lead to models more useful to administrators.

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1. Mancini, John L., 1978, "Numerical Estimates of Coliform Mortality Rates Under Various Conditions," Journal WPCF, 50, No. 11, p. 2477-2484.

2. Thomann, Robert V., 1979, "Measures of Verification," National Workshop on Verification of Water Quality Models, EPA, in press.

VERIFYING A WATER QUALITY MODEL

By

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Cambridge, Massachusetts

This paper presents an example of verification of a Water Quality Model. To facilitate a consistent analysis, the officials of EPA Region III implemented Qual-II Model to perform waste allocation analysis of the Lower Kanawha River, which had experienced low dissolved oxygen in summer and fall. Oxygen consumption was thought to be caused by the carbonaceous BOD and nitrogenous oxidation; resident industries were the major contributors of the organic nitrogen. The model was calibrated by historical data, including 1973 conditions, which had a stream flow slightly higher than $7Q_{10}$ and a Nitrogenous oxidation rate estimated at 0.04/day. An intensive survey was conducted in 1974 to obtain data for model verification. In this survey some interested parties suggested that the normal second stage of biochemical oxidation of organic nitrogen did not occur in these reaches and thus did not need to be removed in treatment plants prior to discharging in this locality.

After analyzing the data and carrying through a variety of statistical tests, we came to the conclusion that the suggestion mentioned above was without merit; it was not supported by the available data for the Kanawha River. We find that parameter values predicted for the Qual-II model were justified. The salient points of this conclusion are summarized below.

1. The size, shape and flow characteristics of the Kanawha River of the reaches near Charleston, West Virginia are much the same as reaches in many other navigable rivers originating in the Appalachian Mountains in which nitrogenous wastes are discharged and are subsequently oxidized in the stream, with the production of nitrate nitrogen. In fact, some of these streams such as the Ohio and Potomac Rivers, were among those in which the normal course of the nitrogen cycle in streams was first demonstrated. Data pertaining to reaction velocity constants for nitrification compiled in standard sanitary texts and handbooks which have been used for many years

are based in substantial part upon extensive stream surveys of this group of rivers.

2. It is known from many laboratory experiments -- bottle tests and model streams - that biochemical oxidation of ammonia and common organic nitrogen compounds to nitrite and nitrate nitrogen will occur if favorable conditions are present. These include: (1) presence of appropriate seeding of autotrophic microorganisms, including Nitrosomonas and Nitrobacter and similar bacteria; (2) adequate time for the reaction to occur; (3) a benign ambient aquatic environment -- pH, dissolved oxygen temperature, ionic strength, etc. Moreover, it is known that nitrification may be inhibited or precluded by unfavorable conditions, such as the presence in active form of some heavy metals (e.g., mercury, chromium and copper) and by the simultaneous occurrence of certain other biochemical processes at high levels of activity that make the aquatic environment unsuitable for nitrification. The latter form of inhibition may occur in heavily polluted streams.

In the first phase of our analysis we examined hydrological, hydrographic, and water quality data from past years pertaining to the Kanawha River and also chemical and physical data pertaining to wastes discharged to the river between stations at River Miles 67.7 to 69.7. Our conclusion is that in general stream conditions are favorable for nitrification at low to moderate rates. No facts or factors were identified that would lead us to conclude that nitrification would likely be inhibited in these reaches.

In the second stage of our analysis we analyzed data recently obtained regarding the fate of nitrogen compounds in the stream with the view of delimiting as closely as possible the amount of nitrogenous oxidation actually occurring in the lower reaches of the Kanawha River under present conditions.

3. One relevant condition for believing that stream nitrification occurs is laboratory demonstration that samples of the nitrogenous wastes do in fact undergo the second stage of biochemical oxygen demand in bottle tests under controlled conditions. Data obtained by EPA Region III analysts amply demonstrate that wastewater samples do oxidize with the production of nitrates. Further, analysis of the laboratory data indicates that the schedule and degree of nitrification is typical of that found with many nitrogenous wastes. Least squares fitting of the data yielded reaction velocity parameters (0.10 to 0.25 per day; Napierian base) that fall within the range found in numerous bottle and model stream tests. The fact that oxidation of nitrogenous compounds of the waste being discharged into the Kanawha River are oxidized under laboratory conditions, of source, does not prove that such oxidation occurs in the river, but it does support a presumption of stream

nitrification unless specific factors in the stream that inhibit second stage oxidation can be identified.

4. The next phase of our investigation pertained to analyses of sets of water quality data from river samples collected twice daily from September 24th to October 3rd, 1974. These 20 sets of data relating to dissolved oxygen and various forms of nitrogen, together with information regarding river runoff and water temperature, were analyzed in several ways to assess the rate and extent of nitrification in the stream.

The reaches of the Kanawha River under consideration extend from River Mile 73.7 at Chelyan Bridge to Mile 58.7 at South Side Bridge. In this 15-mile stretch there are no tributaries of consequence. The Marmet Lock and Dam is located midway at Mile 67.7; this structure, which is just downstream from major wastewater outfalls, speeds the vertical and horizontal dispersion of wastes over the entire cross-section. A large industrial plant and three small communities, Chesapeake, Belle and Marmet, are located on the banks and discharge wastewater effluents into the river. Wastewaters from Chesapeake and Marmet receive primary treatment, Belle's wastewater is processed in an extended aeration plant. All three municipal treatment plants have design capacities of less than 300,000 gallons per day; their contribution to the total flux of pollutants in the river is minor, and the amount of nitrate nitrogen contributed by them is negligible. Wastes from the industrial plant are released through several outfalls between stations at River Miles 68.5 to 69.2. These wastes constitute a major addition to the total flux of nitrogen compounds in the Kanawha River. During the sampling period in late September and early October industrial waste inputs from these outfalls increased the total flux of nitrogenous wastes in the stream by more than 50 percent. Data available to us indicate that during the period of investigation the amount of nitrate nitrogen discharged from the outfalls was very small in relation to the amount of ammonia and organic nitrogen discharged.

During the sampling period water temperature averaged about 20°C with only minor variations. Flow rates in the Kanawha River at this time averaged about 5600 cubic feet per second - almost twice the design flow of 2890 cfs (7-day; 90 percent dry year flow). The mean flow-through time of the 15-mile section was about two days. Runoff was not uniform during the period; higher discharges occurred toward the end of the sampling period (September 30, October 2 and 3, 1974). Because of irregularity of runoff rate, with concomitant fluctuations in velocities and rates of longitudinal dispersion of the wastes, it was not possible to assess accurately the rate of oxidation of ammonia and organic nitrogen for each of the 20 sample sets. Instead it was expedient to amalgamate the data and to compute the average flux rate of the various forms of nitrogen over the entire sampling period. In Table 1 flux rates are shown for

TKN, NH_3, NO_3, Org N and total N. Input to the reach above the industrial wastewater outfalls is calculated as the average flux rates obtained from the water quality data, and stream flow rates at stations at River Miles 73.7 and 69.7. Output of the reach is calculated by similar information from stations at Mile 61.0 and 58.5 below the waste outfalls. Average flux rates calculated in this way together with the standard deviations in flux rate from sample to sample are summarized as follows:

TABLE 1

	Input 10^3 lbs/day (as N)	Output 10^3 lbs/day (as N)	Percent Increase
Nitrate nitrogen	28.8 ± 2.3	32.1 ± 2.3	11
Ammonia nitrogen	3.5 ± 0.6	16.0 ± 0.7	357
Organic nitrogen	9.5 ± 1.2	18.5 ± 2.0	95
Total nitrogen*	41.8 ± 3.2	66.5 ± 4.3	59

*Organic and inorganic, but not including nitrite nitrogen for which no data were available.

The observed increase in the flux rate of nitrate nitrogen based on 39(1) input and 39(1) output samples is 3.3 x 10^3 pounds per day. Since input of nitrate nitrogen from the waste outfalls in the reach during the sampling period was negligible, the observed increase can only be due to (i) nitrification in the stream, (ii) sampling error, or (iii) a combination of (i) and (ii). On the hypothesis that the Kanawha River has nitrifying characteristics similar to those of rivers of the same size with similar pollution loading, one would expect a small but significant amount of nitrate production in the 15-mile reach in a two-day residence time. Such an increase could be measured without difficulty in many situations. In the Kanawha River, however, a large nonuniform flux of nitrogenous material from antecedent pollution occurs as an input to the reach of concern and obscures interpretation of the test results. This variable flux from waste effluents of upstream municipalities and industries makes it difficult to calculate with precision the rate and extent of oxidation of ammonia and organic nitrogen in the sections of the river immediately above and below Marmet Lock and Dam(2).

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(1) Two stations at upstream and downstream for 40 measures, with one deleted for incompleteness of data.

An estimate of the increase in nitrate nitrogen in the reach based on EPA's Qual II model, and calibrated with data for 1973, is 1800 lbs. per day when the flow rate is 5600 cfs and temperature 20°C. [Simulation yields an increase in nitrate concentration from 0.97 mg/ℓ at the upstream end of the reach to 1.03 mg/ℓ at the downstream end; (1.03-.97) x (8.33) x (5560/1.547) = 1800 pounds per day, with the September-October 1974 river conditions.]

In order to apply some standard statistical tests to draw valid inferences regarding nitrification, let the stochastic variate u denote the increase in nitrate nitrogen over the reach. The observed mean value of u, namely $\bar{u}$, based on results for the 10-day sampling period with 20 sample sets, is 3.3×10^3 pounds per day. The standard deviations of the nitrate flux at the upstream and downstream ends of the reach are 14.3 and 14.1 thousands of pounds per day respectively. According to the theory of a widely used statistical technique(3) appropriate for tests of this type, the quantity

$$t = \frac{\bar{u} - E(u)}{S/\sqrt{n}} = \frac{(3.3 - 1.8)}{\left[\frac{(14.3)^2}{39} + \frac{(14.1)^2}{39}\right]^{0.5}} = 0.47$$

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(2) A major component of the antecedent nitrogenous waste derives from a large arsenal about 60 miles upstream. While the waste discharge permit for this source of pollution allows a release of 43,000 pounds of nitrate nitrogen per day, a much smaller amount, about 18,000 pounds per day, was actually discharged during and immediately prior to the sampling period. This actual release was about 10,000 pounds per day smaller than the observed influx to the reach in question (28,800 pounds per day of nitrate nitrogen). The buildup of about 5 tons per day of nitrate nitrogen in the upper reaches of the stream is another indication that the nitrifying characteristics of the Kanawha River are not unusual or abnormal among impounded streams of this class.

(3) See, for example, "Engineering Statistics" by A.H. Bowker and G.J. Lieberman, (Prentice Hall, 1959), pp. 174 and 221; also Appendix Table 3, page 558.

is a stochastic variate distributed in accordance with a student's frequency distribution with $u = 78$(4) degrees of freedom. $E(u)$ denotes the population mean of the u-values. According to the statistical theory, the variate, t, is a dimensionless measure of the deviation of the observed mean from population mean. It has an expected value of zero and a standard deviation of 1.013. If many replicate series of 20 samples sizes were obtained for this reach of the Kanawha River under similar conditions of flow, temperatures, and pollution loading; and if a t-value were computed for each series of twenty samples, it would be expected that the overall average value of t would be close to zero. But owing to random sampling fluctuation, some large values and some small (negative) values would occur. Using tables of the student t-distribution it is possible to calculate the probabilities (frequencies) associated with t-values of different magnitudes. For example, the t-value of 0.47 calculated above under the hypothesis that $E(u) = 1.8 \times 10^3$ pounds per day - a level based on a nitrification velocity constant typically found in streams of this size and hydrological class - would, according to the theory, be exceeded in about one third of the hypothetical replicate sampling series $[Pr\{t > .47\} = 0.319]$. Thus, a value of t of 0.47 (and $\bar{u} =$ 3,300 lbs/day) is not at all incompatible with a true mean u-value of 1800 lbs/day.

If we now test as an alternative hypothesis the suggestion that no biochemical oxidation of ammonia or organic nitrogen occurs in the reach, a t value of 1.03 would be obtained:

$$t = \frac{(3.3-0)}{\left[\frac{(14.1)^2}{39} + \frac{(14.3)^2}{39}\right]^{0.5}} = 1.03$$

From tables of the t-distribution with 78 degrees of freedom, it is found that a t value as large as 1.03 would occur on the average only once in about six of the hypothetical replicate sampling series $[Pr\{t > 1.03\} = 0.153]$. While this is not a rare event, it is significant to note that the probability is only about one-half the probability of the result obtained in the first computation based on the hypothesis that $E(u) = 1800$

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(4)
$$\nu = \frac{\left(\frac{14.1^2}{39} + \frac{14.3^2}{39}\right)^2 (39+1)}{\left(\frac{14.1}{39}\right)^2 + \left(\frac{14.3}{39}\right)^2} - 2 = 78$$

pounds per day. Thus, while the data do not disprove the hypothesis that nitrification does not occur, they are in fact more nearly in accord with the hypothesis that it does occur and at rates typical of impounded streams of this size.

It will be useful perhaps to restate the above inferences in terms of the Neyman-Pearson statistical test and the concept of Type I and Type II errors.(5) Under the hypothesis (call it H_o) that nitrification does not occur, the critical region for rejection of H_o is

$$|t_c| > t_{\alpha/2,\nu} = t_{.025,78} = 1.99$$

when the Type I error is fixed at 5% ($\alpha = .05$). Since the observed t-value of 1.03 is less than 1.99, the null hypothesis cannot be rejected. But if now we calculate the Type II error, it is found to be large. Under the alternative hypothesis (H_1, say) that stream nitrification does occur, it may be shown that with the frequency rejection criterion computed for $\alpha = .05$, a very large Type II error of 0.92 ($\beta = 0.92$) is obtained. These computations are summarized in the following compilation for two different criteria for rejection ($\alpha = 0.05$ and 0.20).

Type I Error		Power of Test	Type II Error
α	$t_{\alpha/2,78}$	$1-\beta$	β
0.05	1.99	0.08	0.92
0.20	1.30	0.27	0.73

At both levels of α the power of the test ($1-\beta$) is seen to be low, and large Type II errors inhere. Evidently the additional data obtained in September and October 1974 are not sufficiently precise to be decisive on this issue. But in view of the large errors it would be most unwise to conclude that since the null hypothesis cannot be rejected nitrification does not occur in the stream. More data are needed for proof or disproof. In further analysis it would be desirable to include consideration of the entire nitrogen balance on the stream in the reaches of interest. Needed data included more detailed information on industrial wastewater releases.

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(5) In the Neyman-Pearson test a critical region is selected in advance of the test for rejection of the null hypothesis. If the t-value, based on test results, falls in the critical region, then the null hypothesis is rejected. The Type I error (α error) is the present probability of rejecting the null hypothesis in cases where the null hypothesis is correct. The Type II error (β error) may occur when the null hypothesis is accepted; it is the probability that the test result will not fall in the critical region for rejection as it should in cases where the alternative hypothesis is true. Thus the β error is a measure of the hazard of making an incorrect inference when the null hypothesis is accepted.

Summary and Conclusions

Our study leads us to believe that nitrification occurs in the Kanawha River at rates in the range typical of other impounded streams of this size. Available data are not sufficiently detailed to delimit precisely reaction velocities under the varying ambient conditions in the river. Rates of biochemical oxidation of ammonia and other nitrogenous wastes are inherently unstable, and large sampling errors are inevitable. Many factors determine the rate and extent of nitrogenous oxidation. For example, on sunny days most of the ammonia present in the stream may be absorbed directly in the metabolic processes of algae, slowing or halting the production of nitrites and nitrates. In Charleston, West Virginia, in a typical year there are 56 clear days, 192 cloudy days and 118 partly cloudy days. Variations in rates of nitrogenous oxidation from this source and from many other causes make it difficult to define norms and to select appropriate input parameters for computer models that attempt to simulate the natural processes of stream self-purification. These difficulties are severe but they do not obviate the need to attempt to establish reasonable estimates of average nitrification rates under stream conditions expected in the future. It would be a serious mistake to conclude from examination of a limited body of information, from which the occurrence of nitrification cannot be conclusively demonstrated, that nitrification is an insigificant factor. We believe that it is a significant factor affecting the oxygen balance of the stream.

TRANSPORT MODELS

By

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The water resources group at Argonne has been involved in the evaluation of specific types of transport models (both mathematical and physical) in terms of prototype-scale, field data. The environment has been primarily the Great Lakes and the transport processes modeled include the near-source behavior of cooling water discharges, whole-lake circulation of Lake Michigan, and extreme nearshore circulation driven by wind and waves. The following summary comments are drawn from the context of these limited experiences and address, in part, the issues of the data base, model detail, and methods of verification.

The most useful data are those acquired specifically for the evaluation of a given model(s). This would appear to be a truism, but it is not clear that it is always appreciated. It is our experience that familiarity with and planning with regard to the specific nature of model inputs, processes, and outputs are essential to the acquisition of data useful for evaluation purposes. Data gathered in monitoring activities, for regulatory or operational purposes, are usually inadequate substitutes. While monitoring data provide time-series records at a few points in a flow system, they often lack the synoptic scope required for model evaluation.

Measurements for evaluation purposes should include measurements of variables that may affect the transport process even though those variables may not be accounted for explicitly in the model. Our studies of thermal plume models and measurements of plumes in the Great Lakes have indicated this to be particularly important with regard to ambient conditions. Models of thermal plumes rarely are able to account for spatial and temporal variations in the ambient environment, and model input often reflect uniform and steady conditions. Measurements by Argonne of a power plant thermal plume at two different occasions, but under identical discharge, ambient stratification, wind, and depth-averaged ambient current conditions, indicated near-surface isotherm areas were substantially different. Investigation of measurement of the vertical structure of the current showed that the current was nearly uniform in one case and sheared in the other. As model input parameters could not account for this variability, calibration of the model against one set of data would surely lead to poor performance against the other set. In this particular case, had the ambient current measurements been limited to single current meter at middepth, the poor performance may have been attributed to some other model parameter.

Despite our desire for an objective standard upon which to determine "verification," we have found no simple quantitative measure. In fact, we often find ourselves discussing model data comparisons in such subjective terms as circulation patterns or plume shapes. The output simulations of four numerical hydrodynamic models for Lake Michigan were compared, at Argonne by Allender, with time-series current observations at fixed points in the lake. Quantitative comparisons included realtime graphs for fixed locations; power spectra, lake-wide plots of average motion, progressive vector diagrams, cumulatie scalar- and vectored-averaged currents at fixed locations; horizontal scalars averages at various depths, and Fourier norms. The major failing of the models was their inability to simulate time-series currents at a fixed location, yet the simulation of circulation patterns appeared to agree "not badly" with patterns inferred from fixed and satellite observations.

RECOMMENDATIONS TO IMPROVE THE USE OF MODELS IN DECISION-MAKING(1)

By

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Modeling techniques have been applied in a variety of subject areas in addition to urban water planning. Recent surveys have discussed the use of modeling in planning (Lee 1973), environmental decision-making (Holcomb Research Institute 1976), and social-human decision-making (Fromm, et al. 1975). Interestingly, the major obstacles to greater use and impact of modeling on decision-making are the same for these topics and for urban water planning. They are:

data availability
modeler-decision maker interaction
model documentation
understanding model assumptions and limitations

For urban water systems, modeling is an area where technology is far ahead of our ability to apply it. Although areas such as ecologic modeling, nonpoint pollution, sediment/solids transport, and water-related economic impacts require further research, current models are limited largely by the data available to calibrate, verify, and apply them. In a survey of project directors and monitors of federally supported modeling activity in social-human decision making, Fromm, et al. (1975) note that data availability was the limitation most often mentioned. Sonnen, et al. (1976) provide a similar conclusion for urban runoff modeling. From our questionnaire survey results, 48 percent of the respondents recommended additional data collection to improve urban water planning while an even larger percentage (57 percent) of the model-using agencies so responded. In each of our case studies data collection efforts accompanied the modeling work.

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(1) Excerpted from "Planning and Modeling in Urban Water Management" by A.S. Donigian Jr. and R.K. Linsley. Hydrocomp, Inc., Palo Alto, CA. Prepared for OWRT. Contract No. 14-34-0001-6222. October 1978. 158 pg.

Although data requirements for modeling depend on the specific water problem and the model being used, Table 1 summarizes the general categories of needed data and provides examples of each. Obviously all models do not require all types of data shown in Table 1, and the examples listed are most directly applicable for simulation models which are the most frequently used types. However, the amount of data required will vary considerably, from information on a single storm event to continuous data for many years depending on the type of analysis performed and the specific information needed for informed planning.

Observed quantity/quality data for streams and receiving waters are most often lacking, and water quality data collection is especially expensive. Data from nearby or similar watersheds may be used in some cases assuming that conditions are similar in both areas. Since the data are used to evaluate model parameters and calibrate the model to local conditions, some local site-specific data are usually needed to insure model accuracy.

The Holcomb Research Institute (1976), in studies for the United Nations Scientific Committee on Problems of the Environment, found that successful model applications in terms of impact on decision-making usually involved extensive interation between modelers and decision-makers. This communication is difficult to establish due to differing backgrounds, objectives, and reward systems. It is a necessary link if the model is to provide the information that the decision-maker needs for the specific problem he is facing. Although our case studies always included users (modelers) within the agency, this did not always insure that the modeling impacted the decision-making process. The Holcomb report recommends (1) regular meetings between modelers and decision-makers to insure agreement on problem definition and needed information, (2) graphics displays to communicate modeling results in semi or non-technical terms, and (3) "policy analysts" with knowledge of both modeling and decision-making processes to further insure effective communication. Our analysis confirms these recommendations.

Many more models are developed than are actually applied for their intended purposes. Although no reliable data exists, Fromm, et al. indicates that "...at least one-third and perhaps as many as two-thirds of the models failed to achieve their avowed purposes in the form of direct application to policy problems." (p. 4, 1975). We would expect similar results for urban water models. Lack of adequate documentation is a major obstacle, especially when models are developed for outside (non-developer) users. Often funds are not allocated or are depleted before documentation is developed. Models are often released without sufficient testing and incomplete or insufficient documentation to decipher program "bugs" that

TABLE 1

DATA NEEDS FOR MODELING URBAN WATER SYSTEMS

Category	Examples
Watershed/System Data	Topographic maps, land use, soils characteristics, pipe network description (length, slope, roughness), reservoir operation, pumping schedules, drainage description, channel dimensions, storage capacities
Meteorologic Data	Precipitation (storm events and/or many years), pan evaporation, maximum and minimum air temperature, other (wind, solar radiation, etc.) as needed.
Observed Water Quantity/Quality Data	Streamflow, lake levels, tide levels and cycles, bay/estuary circulation patterns, concurrent water quality data (for all constituents of interest), urban runoff data (quantity/quality)
Economic Data	Water use (residential, commercial, industrial), flood depth-drainage information, construction cost, treatment cost, O & M costs, recreational use, interest rates

invariably occur. University researchers in modeling usually publish thesis, articles, and reports without recognizing the need for user manuals. Government developed models may or may not include user manuals, but continuing support, user assistance, and program maintenance is almost nonexistent. Models developed on one computer system may not run on another system (even with the same model computer) without program modifications. Thus, adequate documentation should include discussion of theory, assumptions, limitations, and extent of testing/verifying the model, in addition to basic information on program structure, operating instructions, and compatability with other computer systems. Supplementary information would include data requirements, data sources, and guidelines for evaluating model parameters and analyzing model results.

Lack of understanding of model assumptions and limitations is a major obstacle to greater use and impact of modeling especially for decision-makers and non-developer model users. Obviously this is a part of the modeler/decison-maker interaction discussed above, but focuses directly on the model and what it represents. A model is a representation of reality, not a one to one map; it is based on a series of assumptions within which a problem is analyzed. Sonnen, et. al. states that a modeler attempts "...to approximate a solution to a theoretical problem with both an approximation of the theory and an approximation of the prototype water body. The model user or the user of the model's results views his problem, and the theoretical statement, as precise and infinitesimal." (p. 59, 1976).

These conflicting views between the modeler and the user must be resolved if modeling is to be used effectively. The reports by Sonnen, et al. Holcomb Research Institute, and Fromm, et. al. agree that the most successful model applications often include the model developer as the user. In seven of our eight case studies the agencies either developed model components or were assisted by the model developers. Involvement in the model development process requires the user to be acutely aware of model assumptions and limitations, and thus allows him to most effectively interpret and analyze the model output. Without this understanding, the model may be analyzing a problem different from, or considerably simpler, than the one the decision-maker faces.

A related obstacle results from the impression that in a modeling study the model is the sole guide to decision-making. It must be kept in mind that "...a model is a means to an end, and not an end in itself." (Lee 1973, p. 19). The real analysis begins when the model run is finished because the interpretation of the modeling results is the critical step in the modeling study. Even with optimization models which produce a socalled "optimal" plan, project design, or policy, the final recommended plan will likely be different from the optimal plan because of the many other inputs to the decision-making process.

From the questionnaire survey, the case study investigations, and our analysis of the urban water modeling field, the following recommendations are extended to potential model users and decision-makers to help improve the use and effectiveness of modeling in decision-making:

(1) Require a detailed definition of the problem and the specific information to be provided by the model. The problem definition may be part of the modeling study. Otherwise, the problem should be clearly defined and the type of information provided by the model and the analyses to be performed should be specified.

(2) Develop close modeler-decision-maker interation. Throughout the modeling and analysis phases of a modeling study, regular meetings between the modelers and decision-makers should help to develop effective two-way communication. If modeling consultants are employed, a staff person should be assigned liaison between consultant and decision-maker and be thoroughly familiar with the model and the modeling application.

(3) Use existing models to the extent possible. A review of available models should be conducted to evaluate appropriate models. Consultants may assist in this process but the final choice should depend on the user's understanding of the problem, the model assumptions and limitations, and the analyses to be performed. Model development may be required if no models appropriate to the problem are available. However, modifications to an existing model are usually more cost-effective than developing a completely new model.

(4) Require adequate documentation. Adequate documentation includes discussion of theory, assumptions, limitations, and extent of testing/verification in addition to basic information on program structure, operating instructions, and compatibility with various computer systems. Supplementary information includes data requirements, data sources, and guidelines for evaluating model parameters and analyzing model results. If the model is being developed or modified, installation on the user's computer facility should be required.

(5) Require complete delineation of model assumptions and limitations. The way the model represents the system,

including simplifying assumptions and resulting limitations, must be clearly explained so that the decision-maker understands what the model can and cannot do.

(6) Integrate modeling and data collection efforts. Most modeling applications will require some data collection often involving monitoring, sampling, and analysis. Such programs should be integrated with the modeling so that the specific data required by the model is supplied.

If data requirements and/or collection are extensive, a data management (computer-based) system may be needed to efficiently store, retrieve, verify, and prepare the data in a form suitable for modeling.

(7) Emphasize analysis and preparation of model results. Sufficient resources must be allocated to the analysis of the model results to insure that the information produced is usable by decision makers. This is the key step that determines whether or not the modeling results will impact the final plan, project, or policy recommended.

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SALINITY MODELS APPLIED IN THE ARID WEST

By

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Over 80 percent of the flow of the Colorado River originates from snowmelt and rain in the high mountain watersheds. This high quality water accumulates total dissolved solids (TDS, salinity) rapidly as it flows into and through the lower elevation arid regions of the basin. For example, TDS in the Price River, Utah at a flow of 50 cfs has been observed to increase from 300 mg/l to over 3000 mg/l in a distance of 50 miles (Dixon, 1978).

Traditionally, the extensive deposits of Mancos shales have been considered the prime source of TDS in the Upper Colorado River Basin. They are marine deposited shales intermixed with lenses of sandstone and limestone. Soils derived from them are typically saline. Several processes are thought to contribute to the increase in TDS concentrations as the water flows downstream: 1) a portion of the stream water moves from the channel into the salty alluvium and back into the channel again; 2) groundwater percolating through salty formations; 3) irrigation return flow (surface, interflow, deep percolation); 4) efflorescence in intermittent stream channels which is periodically flushed out by thunderstorms; 5) salt pick-up by overland flow (sheet flow and flow in rills); 6) salt associated with eroded soil; 7) reservoir evaporation; 8) evapotranspiration (agricultural and natural); 9) export of high quality water out of the basin; 10) industrial, energy, and municipal development. The precipitation of salt has been observed in reservoirs and some stream channels.

The characteristics of a variety of models applied to salinity problems in the arid West are summarized in the Table. The purposes of these models have been: 1) to evaluate impacts of energy and agricultural development on downstream salinity and; 2) as research tools to identify and quantify TDS contributions from the various processes.

MODEL CHARACTERISTICS

REFERENCE	MODEL TYPE	TIME INCREMENT	CONSTITUENTS	MODEL PROCESSES	APPLICATION
Hyatt, et al. 1970	Watershed, deterministic	Monthly	Total dissolved solids (TDS), (conservative)	Agricultural runoff and interflow (crop consumptive use, irrigation efficiency) natural system surface runoff, groundwater flows, interchange between surface and groundwater.	38 subbasins of the Upper Colorado River Basin.
Thomas, et al. 1971	Watershed with soil column under agricultural land. Deterministic processes.	Monthly	Ca, Mg, Na, SO_4, Cl, HCO_3 (nonconservative)	Agricultural runoff and interflow (crop consumptive use, irrigation efficiency), natural system surface runoff, interflow groundwater flows, specific ion precipitation and dissolution in the agricultural soil profile.	Little Bear River Basin, Utah.
Ribbens and Wilson, 1973. Colorado Salinity Control Forum, 1975.	River system network, deterministic	Monthly	TDS (conservative)	Each subbasin is represented as a node in a river system network. The time varying (monthly) effects of agriculture (irrigation practices) energy development, natural systems, point loads and diversions are input at each node and water and salinity balances are conducted on the network. Reservoir operations.	Lower Colorado River Basin.
Utah State University 1974 a,b,c.	In-channel, deterministic water quality model	Steady-state during critical flow periods.	TDS (conservative)	Point loads and diffuse sources along the river system.	Bear, Virgin and Sevier River Basins in Utah.
Hill, et. al. 1973; Hill, et. al. 1975; Utah State University 1975 Israelsen, 1979	Watershed, deterministic	Monthly	TDS (conservative)	Agricultural runoff and interflow (crops consumptive use, irrigation efficiency), energy development, natural system surface runoff, groundwater flows, interchange between surface and groundwater.	Bear River Basin San Juan River Basin Palo Verde, California Sevier River, Utah

MODEL CHARACTERISTICS

REFERENCE	MODEL TYPE	TIME INCREMENT	CONSTITUENTS	MODEL PROCESSES	APPLICATIONS
Utah State University, 1975	River system network, deterministic	Steady-state at specified flows and boundary conditions	TDS (Conservative)	Each subbasin is represented as a node in a river system network. The effects of agriculture (irrigation practices), energy development, natural system, point loads and diversions are input at each node and water and salinity balances are conducted on the network.	Colorado River Basin (Wyoming to Imperial Dam, California)
Narasinham and Israelsen, 1975	Watershed, deterministc	Monthly	Ca, Mg, Na, SO_4 Cl, HCO_3 NO_3 (Nonconservative)	Agricultural runoff and interflow (crop consumptive use, irrigation efficiency), natural system surface runoff, groundwater, and interchange between surface and groundwater. Specific ion precipitation and dissolution in the agricultural soil profile.	Twin Falls Tract, Idaho.
White, 1977.	Emperical non-point in-channel loading functions.	Annual	TDS (Conservative) Suspended Sediment.	Salt release to in-channel flows for intermittent flows. Salt-sediment interaction.	Price River Basin, Utah
Jurinak, et.al. 1977	Watershed, stochastic rainfall linked to deterministic processes.	Daily	Ca, Mg, Na, K, Cl, SO_4, P, Carbonates, Zn, Cd, Pb, Cr, Hg.	Stochastic rainfall. Soil chemistry equilibrium reactions for specific ions. Erosion of soil with associated specific ions. Water transport of specific ions by overload flow, infiltration, and soil transport.	Fremont River Basin Dirty Devil River Basin Colorado River Basin Escalante River Basin San Juan River Basin
Ponce and Hawkins, 1978	Emperical non-point overland flow loading functions	Annual	TDS (conservative)	Salt release to overland flow over mancos shale soils.	Price River Basin, Utah.
Dixon, 1978	In-channel, deterministic	Hourly	TDS (conservative)	Unsteady flow routing in the channel. Natural system salinity pickup from in-channel processes.	Coal Creek, Price River Basin, Utah

MODEL CHARACTERISTICS

REFERENCE	MODEL TYPE	TIME INCREMENT	CONSTIUENTS	MODEL PROCESSES	APPLICATION
Chadwick, 1978	Watershed. Stochastic rainfall linked to deterministic process model.	Variable; about hourly during rain events.	TDS (conservative)	Stochastic rainfall, interception, infiltration, evapotransporation, salt release from natural sources to overland flow and to inchannel flow.	Coal Creek Basin and the Price River Basin, Utah
Malone, et al., 1979	River system network, probabilistic	Steady-state at specified flow conditions.	TDS (conservative)	Each subbasin is represented as a node in a river system network. The effects of agriculture (irrigation practices), energy development, natural system, point loads and diversions are input at each node and water and salinity balances are conducted on the network. Uncertainties (variances) associated with salinity sources are also input at the nodes and propagated through the system.	Colorado River Basin (Wyoming to Imperial Dam, California)

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TRANSPORT ON THE CONTINENTAL SHELF IN THE NEW YORK BIGHT

By

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The New York Bight is a section of the continental shelf extending from Montauk Point at the tip of Long Island to Cape May at Delaware Bay, and out to the 200 m isobath. A multidisciplinary investigation of the Bight has been going on since 1973 under the NOAA/Marine Ecosystems Analysis Program. The physical oceanography part of the program which is directed by Dr. Donald V. Hansen and myself at AOML, includes measurement of temperature and salinity at over 80 stations, 4 to 5 times per year, as well as concurrent dissolved oxygen and nutrients measurement in cooperation with Dr. Atwood of AOML. Arrays of recording current meters have been deployed throughout the Bight to look at nearshore flow, (depths less than 30 m) dispersion from the Hudson River plume and shelfwide general circulation. Over 65 current meteryears of data have been gathered since 1973.

One of the major efforts of the program is a multi-parameter model of the carbon/oxygen/nitrogen cycling in the Bight being developed by Dr. John Walsh of Brookhaven National Laboratory. The transport field for this model is provided by a diagnostic model developed by Dr. Jerry Galt and applied by me to certain specific flows which are observed in the Bight.

Transport on the Continental Shelf has certain characteristics which require different treatment than in estuarine and riverine systems. The major flows on the shelf, other than the tidal oscillations, are alongshore barotopic responses to the alongshore windstress. The flow is geostrophically balanced with the across-shelf sea surface set up induced by Ekman surface layer transport. It is not directly forced by the friction at the sea surface except very near the coast at depths less than about 30 m. The flows are oscillatory at the frequency of storm occurrance (3-10 day period) with magnitudes of up to 50 cms^{-1}.

The mean flow is southwestward with a mean velocity of 1-5 cms^{-1} which is very small compared to the oscillations. Even this small mean velocity results in an alongshore transport of 20 x $10^5 m^3 s^{-1}$ which is 100 times the flow of the Hudson River.

Water quality modeling is hampered by several factors which are:

1) An open boundary along the shelf break across which sharp gradients of nutrients and other constituents are present but about which we have very little knowledge of the mixing.

2) Cross shelf boundaries with large transport which is highly variable both in time and across the section

3) Weak along shelf gradients which makes calculation of the divergence of a constituent flux very inaccurate.

4) Changes in stratification from highly stratified to homogenous which changes the dynamics through the year.

5) Mixing effects of breaking internal waves on the outer shelf.

It is the cross-shore mixing of constituents which are input to the shelf from the shore and from nearshore dumping activities which is the most important and the most difficult to specify. The long time scale for cross shore mixing (years) and the input of freshwater from many sources along the shore precludes use of freshwater as a tracer for calculation of mixing coefficients except very near the river mouth. The Hudson Shelf Valley appear to act as a conduit for cross shelf transport of clean outer shelf bottom waters into the area at the mouth of the Hudson River (commonly called the Bight Apex).

Because of all these problems we have kept our initial goals for the water quality model modest. Nature was kind in providing an event in 1976 which has enabled us to test the model's capabilities. The so-called "anoxia" event in May-September, 1976 produced large gradients in space and time and a large signal in many parameters. A complete description of the event is contained in a forthcoming NOAA Professional Paper. Application of the diagnostic model to the computation of transport across sections of a box model of the layer below the pycnocline, enabled us to calculate the divergence of oxygen flux over 40 days during the development of the event. Thus, we could infer the net utilization of oxygen which was required to produce the observed oxygen decrease. It appears that the respiration of a large concentration of dinoflagelates alone was of the correct order to produce the required utilization of oxygen. Upcoming work with Dr. Walsh will attempt to compare the circulation patterns and biochemical conditions between the 1976 event and the preceding "normal"year. Further studies will focus on events extending from March through the summer of 1975 and 1976 since it is hypothesized that the bloom of dinoflagelates were instituted by conditions present early in the year. The presence of a deep pycnocline formed by a warm, early spring favored the growth of the heterotrophic species over the autotrophic nanoplanketon which typically succeeds it each spring.

The diagnostic model is a vorticity balance model with linear bottom friction which requires an input of observed density, bottom topography and the barotrophic velocities perpendicular to the boundaries. Output is the barotrophic velocity field over the entire region. Solution is done with a finite element technique. Solid boundaries are defined by a no flux condition on the boundary solution. Baroclinic velocity shear in the vertical is assumed geostropic except for the top and bottom Ekman layers. The complete velocity profile is calculated using a turbulance closure scheme model of Mellor and Durbin. Transports are easier to specify. Top and bottom flow, as separated by the pycnocline, is found by integrating the geostrophic transport over each layer and then assigning the Ekman transport to the proper layer.

The model resolves storm events by selecting the time average of the observed velocity at the boundaries over the proper time period to resolve the storm drive flows. Thus, successive time periods have dramatically different flows which are often oppositely directed. Resolving the structure of these advective flows in both time and space minimizes the transport forced into the diffusive or unresolved part of the transport.

Some parameterization of diffusive processes is still necessary. We have calculated the cross shelf horizontal (K_x) and cross pycnocline vertical (K_z) eddy diffusivities by tracing the decay of the well known "cold pool" of winter water. In May of each year cold, salty water with temperatures down to 20°C moves through the Bight at a rate which is observed by current meter measurements. The change in T-S properties is consistent with $K_x = 4 \times 10^6 \text{ cm}^2\text{s}^{-1}$ and $K_z = 0.02$ to $0.1 \text{ cm}^2\text{s}^{-1}$ as found by solving the salt and heat balance equations simultaneously. Mixing in the apex was also studied using an estuarine type salt balance model. This shows a flushing time of 6.8 days, which confirms Ketchum's earlier estimate.

We are attempting to model the transport of dissolved and suspended constituents on the continental shelf using a combination of old and new techniques to approach a difficult problem. Verification of the model is an important step in making the model useful for planning studies. The great quantity and diversity of data which has been collected over the past 5 years will allow us to effectively address the difficult questions of transport and water quality in the New York Bight.

THE ROLE OF WASTE INFLOWS AND LANDSAT IMAGERY IN MANAGING LAKE QUALITY

By

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Introduction

During the last 15 years, substantial progress has been made in cleaning up point sources of pollution and their immediate downstream impact. As a result, secondary impacts to water quality are receiving more attention. This includes the impact of both point and nonpoint sources on lakes and reservoirs (e.g., the EPA Clean Lakes Program). Unfortunately, the dynamic nature of lakes and reservoirs makes it difficult and costly to monitor quality variations, define desirable conditions, and establish cause and effect relationships. In order to formulate effective management plans, improved techniques are needed for relating waste inflows to relevant characteritics of lake quality and for economically obtaining the data required for decision-making. This paper briefly discusses the use of inflow/outflow models and Landsat imagery in meeting these needs.

Waste inflows represent control variables which, hopefully, can be managed in a manner consistent with water quality and other objectives. Comparative data, such as that provided by remote sensing, is useful in isolating problem areas, developing priorities, monitoring improvements, and in separating natural phenomena from man-induced impacts. Mathematical models aid the interpretation of this information for management purposes. Two particular types of models are discussed here: the first relates waste inflow to lake quality; and the second relates satellite imagery to lake quality.

Waste Inflows and Lake Quality Impacts

In recent years substantial research has been devoted to defining lake quality in terms of trophic state indices and relative classifications (e.g., Shannon and Brezonik, Carlson, Ott). Numerous models have been developed to relate quality factors and trophic status to waste inflow, hydraulic conditions and other relevant variables. These range from simple empirical models (e.g., Vollenweider, Dillon, and Rigler, Larsen and Mercier) to complex mechanistic models of the interactions between a variety of ecosystem components (e.g., Chen and Orlob, Leidy and Jenkins, Park). Although these indices, classification systems, and models are useful in many types of analyses, a complete methodology is generally not available for defining acceptable waste loads, water quality standards, and cause-effect relationships.

Simple trophic state indices and empirical response models have proved useful for some decision-making purposes, but fail to include the impact of many important variables (e.g., other waste inflows, meteorology, flow patterns, and spatial and seasonal variations). Complex ecosystem models which include many of these factors are difficult to use and require extensive data. Their cost and sophistication often makes them inappropriate for routine use.

This situation suggests the need for a new generation of predictive empirical models. These new models would have a level of sophistication somewhere between simple empirical models and complex ecosystem models. They would not replace existing models, but rather, complement them. They would be specifically designed to facilitate management decisions by relating controllable waste inflows to those lake conditions which directly impact beneficial uses. They should include the important physical dimensions and causal factors, but should not be excessively complex or costly to use. They should relate inflows of potential pollutants, such as nutrients, organic wastes, toxic substances, and suspended solids, to relevant quality characteristics, such as trophic status, dissolved oxygen concentration, algal growth, clarity, pathogenic organisms, and toxic impacts. They should also include the relevant effects of factors, such as hydrodynamics, geometry, meteorology, and spatial and seasonal variations.

These criteria might seem to imply the need for integrated ecosystem models similar to those already developed. This is not the intent, however. The objective is, rather, a set of specialized models for individual measures of lake quality. Each model would include only those factors most important to the process or condition being considered. Obviously, this is an ambitious objective which has been partially addressed by many researchers. Future needs, however, suggest increased emphasis.

Landsat Imagery and Lake Quality Monitoring

Managing lake quality requires a variety of data, as suggested by the waste inflows, quality characteristics, and causal factors mentioned above. Much of this data must be obtained through detailed field surveys. The cost of these surveys, however, makes it impractical to routinely monitor spatial and seasonal variations in a large number of reservoirs. Fortunatly, there are alternative methods for collecting some of the comparative data needed for managing lake quality. One promising alternative is Landsat imagery. There are presently two functioning Landsat satellites. They provide coverage of a given area every nine days. Each satellite is equipped with a multispectrao scanner which records reflected radiation from the earth's surface for four spectral bands. Each image value represents a 57 x 79 meter, picture element of the earth's surface.

Using this satellite data for water quality management requires regression models relating the image values (or derived statistics) to relevant water quality parameters. For example, ground truth data for chlorophyll concentrations, secchi disc depth, turbidity, or nutrient concentrations, can be related directly to the satellite data, or combined to form indices which can be related to the satellite data. If a set of reliable models or relationships can be developed, future satellite data can be used to routinely monitor these measures of lake quality.

Boland, Scarpace, and others have demonstrated the feasibility of this technique for trophic classification of lakes and for specialized types of water quality monitoring. Although the quality parameters and water depths which can be examined are limited, the low cost and the spatial and temporal range of satellite data allow a variety of comparative analyses (e.g., spatial and seasonal variations within one lake; relative comparisons of separate lakes; and routine monitoring of long-term trends). The results will be useful in identifying problem lakes, in setting priorities, and in establishing regulatory standards.

Specific areas for further work include: (1) acquiring better ground truth data; (2) correcting Landsat data for atmospheric absorption, scattering, and sun angle changes; (3) applying these techniques to a broader set of lakes, reservoirs, and management problems; and (4) developing a more standardized set of models and model variables.

Summary

It appears that greater emphasis will be placed on managing lake quality in the future. This will require greater quantification of the impact of waste inflows on lake quality and more economical methods of obtaining routine data. In order to meet these needs, greater emphasis should be placed on the developing and applying of inflow/outflow models and Landsat monitoring techniques.

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URBAN WASTELOAD GENERATION BY MULTIPLE REGRESSION ANALYSIS OF NATIONWIDE URBAN RUNOFF DATA

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Mechanisms of Wasteload Generation

Nonpoint source loads of pollutants to receiving waters are by definition generated by mechanisms in which the land surface is both the source and initial conveyance of the water quality parameters. As stormwater is routed through the drainage system, further material may be generated or lost through processes of scour and deposition, particularly in combined sewer systems.

Generation of pollutants (e.g., suspended solids) from both the land surface and drainage channels is a problem of sediment transport that is poorly understood even after decades of research. For instance, it is not clear what mechanism apply on the land surface since erosion may be achieved both through the impact of raindrops (e.g., the Universal Soil Loss Equation Approach) and through the boundary shear of overland flow (e.g., the sediment transport approach). In the former case, it is difficult to separate "buildup" and "washoff" relationships, while in the latter case it is popular to assume for modeling purposes that pollutants are "generated" by some mechanisms during dry periods and are available to be washed off by stormwater runoff.

There is considerable current research underway to determine the underlying physical and chemical mechanisms at work in generation of nonpoint source loads. This task is made all the more difficult by the fact that it is seldom possible to separate "buildup" and "washoff" mechanisms strictly from measurements of flow and concentration at a catchment outlet.

Regression Approaches

One alternative to conceptual or physically based models is to perform a regression of measured loads at catchment outlets versus hydrologic, demographic and other relevant factors. Either an arbitrary (e.g., multiplicative) model may be used or a fit of an assumed (e.g., sediment rating curve) model may be made. This approach has been used in numerous urban runoff studies; thirteen examples are summarized by Smolenyak (1). Correlation is often questionable due to the low number of data points available and the frequent presence of spurious correlation when loads (concentration x runoff volume) are regressed against runoff volume.

Regression of Nationwide Data

This synopsis describes briefly the results of such a study performed on extensive data contained in the EPA Urban Rainfall-Runoff-Quality Data Base (2,3). Data from 22 catchments in 12 cities were analyzed by stepwise multiple linear regression (1). Dependent variables were loads (e.g., lb/ac) on a per storm basis for several parameters.

Independent variables included the following:

AVRAIN - Average rainfall intensity (in/hr),
FLOW - Flow volume (in),
PDD - Preceding dry days,
PFLOW Peak flow rate (in/hr),
PRAIN - Peak rainfall intensity (in/hr),
PADUR - Rainfall duration (hr), and
RAVOL - Rainfall volume (in).

It was not possible to include demographic parameters among the independent variables due to the low number of differing land uses among the catchments.

All rainfall-runoff-quality data were first analyzed to determine flow and time weighted concentrations and standard deviations as well as total loads for each catchment for each storm (3). A composite weighted average concentration and standard deviation was also computed for each catchment from all storms. These are shown in Table 1 for parameters BOD_5 and suspended solids. Although combined sewered areas tend to have higher average concentrations than storm sewered areas, no clear distinction among land uses may be made.

When storm event loads were subjected to the stepwise multiple regression analysis described earlier, the most significant independent variables to enter the regression (and the parameters providing the best bi-variate relationship) were as follows.

Table 1 . Comparison of flow-weighted BOD_5 and suspended solids means and standard deviations by land use and type of sewerage (3).

City-Catchment	Storm or Combined Sewerage	00310[a]-BOD_5		Number of Events	00530[a]-Susp. Solids		Number of Events
		Mean (mg/1)	Std.Dev. (mg/1)		Mean (mg/1)	Std. Dev. (mg/1)	
Single-Family Residential							
San Francisco,CA-Selby St.	C	38.1	30.0	8	215.4	146.0	8
Racine,WI-Site I	C	89.6	17.7	7	178.9	137.3	7
Lancaster,PA-Stevens Ave.	C	56.2	49.3	5	271.3	171.1	5
Broward County,FL-Residential	S	6.7	4.3	20	28.4[b]	16.7[b]	28
San Francisco,CA-Vicente St. N.	S	9.8	11.4[c]	1	48.3	29.2[c]	1
San Francisco,CA-Vicente St. S.	S	4.5	3.4[c]	1	45.8	29.3[c]	1
Lincoln,NB-39 & Holdrege	S	37.6	51.8	13	735.9	302.8	18
Lincoln,NB-63 & Holdrege	S	22.1	32.5	11	827.7	228.4	12
Lincoln,NB-78 & A	S	8.7	5.1	9	1532.0	780.4	10
Windsor,ON-Labadie Rd.	S	16.9	8.2	20	389.8	254.2	20
Seattle,WA-View Ridge 1	S	18.4	11.2	7	55.6	102.5	28
Seattle,WA-View Ridge 2	S	12.9	9.4	5	107.7	33.1	4
Seattle,WA-Lake Hills	S	6.3	2.9	5	61.3	9.9	5
Seattle,WA-Highlands	S	4.2	3.8	4	109.3	71.5	4
West Lafayette,IN-Ross-Ade	S	59.6	89.7	8	104.7	52.0	8
Greenfield,MA-Maple Brook	S	11.6	7.2	4	147.4	112.1	5
Multiple-Family Residential							
San Francisco,CA-Baker St.	C	22.9	6.0	3	90.7	14.5	3
San Francisco,CA-Brotherhood Way	C	45.6	24.7	3	654.8	524.6	3
San Francisco,CA-Laguna St.	C	46.3	8.8	2	210.7	101.0	2
Commercial							
Seattle,WA-Central Bus. Dist.	C	64.3	37.7	5	161.8	21.7	5
Seattle,WA-Southcenter	S	12.5	7.7	7	93.5	237.0	27

Table 1 (Continued)

City-Catchment	Storm or Combined Sewerage	00310-BOD_5 Mean (mg/1)	00310-BOD_5 Std. Dev. (mg/1)	Number of Events	00530-Susp.Solids Mean (mg/1)	00530-Susp.Solids Std. Dev. (mg/1)	Number of Events
Industrial							
Seattle,WA-South Seattle	S	11.9	8.2	7	114.2	176.3	29
Mixture-Res., Com., Other							
San Francisco,CA-Mariposa St.	C	43.2	42.5	3	172.4	86.4	3
Durham,NC-Third Fork	S	127.3	13.6	2	1498.3	171.2	4
Northampton,MA-Market St. Brook	S	30.1	19.4	3	149.2	55.0	6

[a] STORET code for parameter. Refer to Table VI-3 in first Data Base Report (2).

[b] Parameter 70299 reported instead of 00530, i.e., suspended solids determined by evaporation instead of filtration.

[c] Standard deviation based on within-storm variation, 8 samples for BOD_5 and 10 samples for SS.

Most Significant Parameters	No. of Catchments
FLOW	9
PFLOW	8
PRAIN	2
RAVOL	2
AVRAIN	1

The predominance of flow volume and peak flow rate is further enhanced by their own significant correlation ($FLOW = 0.262\ PFLOW^{0.77}$, $R^2 = 0.62$, $n = 241$) which may be justified in part on the basis of unit hydrograph theory. Thus, one conclusion of the study is that flow volume is the most significant individual hydrologic parameter in the generation of urban runoff loads. This may be modified somewhat in light of the presence of an un known degree of spurious correlation since loads are computed as a summation (over a storm event) of flows x concentrations and are regressed against a summation of flows (to obtain FLOW).

It was found that, using combined data from all catchments, relationships that are significant at the 99 percent level (F test) could be developed for all dependent variables as a function of FLOW. These are shown in Table 2. In addition most parameters were significantly correlated versus suspended solids (TSS) in a power (log-log) relationship ($0.18 \le R^2 \le 0.83$). This suggests that solids may be used as the basis of prediction of other parameters, a common assumption in surface runoff quality modeling.

As seen in Table 2, the exponent in the equation for TSS is 1.1; individual catchments among the 22 studies produced exponents ranging from 0.72 to 1.3. These values agree well with other urban studies, as shown by Smolenyak (1) and serve to justify the sediment rating curve approach. Exponents in non-urban areas tend to be on the order of 2.0, higher because of the absence of an upper limit on sediment availability.

Of interest is the fact that preceding dry days (PDD) was significant at the 0.95 level for at least one pollutant in the multiple regression analysis for five catchments and was not significant for three others. (It was not available for the remaining 14 catchments). Thus the significance of antecedent conditions in wasteload generation remains unanswered.

Conclusions

Ideally, stormwater runoff loads to receiving waters should be determined by direct measurements. Since this is often impossible due to monetary and other constraints (e.g., the absence of wet weather during the sampling program) generalized results from other studies may be utilized for preliminary estimates. However, all of the customary caveats and

TABLE 2

RELATIONSHIPS BETWEEN POLLUTANT LOADS (lb/ac) AND FLOW VOLUME, (in.) DEVELOPED USING COMBINED DATA FROM 22 CATCHMENTS (1)

Dependent Variable	R^2	Sig. Level F-Test	No. of Events	Model: $\text{Load} = a(\text{FLOW})^b$ Reg. Coefs.	
				a	b
BOD	.28	.99	80	34.0	1.12
COD	.76	.99	157	29.8	1.08
NH3N	.44	.99	20	.215	.72
NITN	.80	.99	21	.119	.80
NTOT	.57	.99	103	.0400	.71
ORGN	.88	.99	40	.856	1.04
TOTN	.74	.99	37	.304	1.07
DOP	.83	.99	34	.0648	.98
TOP	.46	.99	119	.0104	.78
TOTP	.66	.99	53	.426	1.5
TPHOS	.91	.99	8	.105	1.05
TOTS	.69	.99	41	279	1.41
TSS	.56	.99	260	44.2	1.10

Dependent Variable Definitions

BOD-Biochemical Oxygen Demand, 5-day
COD-Chemical Oxygen Demand
NH3N-Nitrogen, Total Ammonia
NITN-Nitrate Nitrogen, Total
NTOT-Nitrite + Nitrate, Total
ORGN-Nitrogen, Total Organic
TOTN-Nitrogen, Total
DOP-Orthophosphate, Dissolved (as P)
TOP-Orthophosphate, Total (as PO_4)
TOTP-Phosphorus, Total (as P)
TPHOS-Phosphate, Total (as PO_4)
TOTS-Solids, Total
TSS-Suspended Solids, Total

precautions pretaining to regression analyses and their use and interpretation are of even more importance here due to the wide variation of measured results and relatively weak data base used to produce the statistical models.

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USGS DATA COLLECTION PROGRAMS RELATED TO WATER QUALITY MODELING NEEDS

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Several ongoing U.S. Geological Survey data collection programs have potential benefit to water-quality modelers. Most modelers find the USGS streamflow gaging network useful and adequate for many of their modeling needs; however, many modelers are not aware of the substantial water-quality data available for water-quality investigations. Some of the major USGS programs that relate to water-quality modeling needs are discussed below. All data is available on the USGS National Water Data Storage and Retrieval system (WATSTORE) or on the National Water Data Exchange (NAWDEX) system.

Fixed Point Monitoring

Fixed point monitoring emphasizes long-term effects. Two networks are operated by USGS. The National Stream Quality Accounting Network (NASQAN) and the Hydrologic Bench Mark program.

NASQAN

The National Stream Quality Accounting Network (NASQAN) is a data-collecting facility for obtaining regional and nationwide overviews of the quality of our streams. Water-quality data from NASQAN stations provide the information needed to:

Account for the water quantity and quality of water moving within the United States;

Develop a large-scale picture of how stream quality varies from place to place; and, Detect changes in stream quality with time.

NASQAN is different from other water-quality monitoring studies in several important ways:

> The network is designed around a system of subdivided river basins, so the collected water data can be related to conditions within a known area upstream, and compared with that from adjacent or nearby areas.
>
> Stations are operated uniformly; therefore, results obtained can be compared directly because the same methods are used to collect and analyze the data at all stations in the network.
>
> Stations are committed to long-term objectives, so the length of record at all stations, the frequency of sampling, and sampling locations will remain uniform for a long time. The uniformity allows for valid comparisons between stations and provides an opportunity to look for long-term changes.

Obviously, it is impossible to measure the characteristics of every drop of water flowing in a stream. Samples, therefore, must be collected from enough places and at the proper frequencies to give a reasonable representation of overall conditions.

The spacing of NASQAN stations is based on a system of hydrologic subdivisions developed by the U.S. Water Resources Council (WRC). In this system, drainage basins in the United States are divided into 21 regions, 222 subregions, and 349 accounting units, the latter two being progressively smaller parts of a region. NASQAN monitoring sites (stations) are located at points chosen to provide a good sample of the water leaving an accounting unit.

To date (1978) 445 NASQAN stations have been established, with a station representing every accounting unit. Ultimately, NASQAN will include about 525 stations in order to adequately cover coastal areas.

A visitor to a typical NASQAN station will first see an instrument shelter about the size of a telephone booth (at some stations, the shelter is several times as large). Inside the shelter is an instrument that obtains a continuous record of stream stage (water elevation), from which streamflow is computed. Many stations also are equipped with a recorder for obtaining continuous data on water temperature and specific electrical conductance; otherwise, conductance and temperature are measured by an observer who visits the site once every day.

In addition to the daily sampling and continuous records that are kept, the following data are collected at each station by a field party:

Twelve times per year (approximately monthly)
Temperature
Specific conductance
  pH (balance between acids and alkalies)
  Bacteria indicators
  Inorganic compounds
  Biological nutrients
  Suspended sediment
  Floating algae
  Organic carbon
Four times per year
  Trace elements
  Attached organisms

Samples for analyses of about 20 pesticide compounds are collected at 153 NASQAN stations. Samples for radiochemical analyses are collected at 51 NASQAN stations at frequencies ranging from monthly to semiannually.

Some of the above measurements are made directly on the stream, but many others require bottling and preservation of samples by icing or addition of chemicals so that consistent analytical results can be obtained after shipment to a laboratory.

The U.S. Geological Survey designed NASQAN, and Survey personnel operate most of the stations and analyze the samples collected. Other agencies, however, such as the Environmental Protection Agency, the U.S. Army Corps of Engineers, and State and local organizations either take part in the operation of some stations or provide financial support. Because of local interests and needs, several agencies usually cooperate in supporting the different parts of a single station.

Information from NASQAN represents one of the important building blocks required for good management of the Nation's waters. It tells us how things are (How much water? What quality?) on a national and regional scale. It represents a baseline against which we can measure the importance of future changes in water quality.

NASQAN data already are being published in annual reports and are being used in making important decisions about the future management of our water resources.

For those who would like to learn more about NASQAN, the Geological Survey has published a more detailed description. Copies may be obtained by requesting USGS Circular 719, "The

National Stream Quality Accounting Network (NASQAN) - Some Questions and Answers." by J.F. Ficke and R.O. Hawkinson, from:

Branch of Distribution
U.S. Geological Survey
1200 South Eads Street
Arlington, Virginia 22202

reference: NASQAN: Measuring the Quality of America's Streams by Benjamin L. Jones, U.S. Government Printing Office, 1978.

Hydrologic Bench Mark Program

Water-quality data, collected at 57 hydrologic bench-mark stations in 37 States, allow the definition of water quality in the "natural" environment and the comparison of "natural" water quality with water quality of major streams draining similar water-resources regions. Results indicate that water quality in the "natural" environment is generally very good. Streams draining hydrologic bench-mark basins generally contain low concentrations of dissolved constituents. Water collected at the hydrologic bench-mark stations was analyzed for the following minor metals: arsenic, barium, cadmium, hexavalent chromium, cobalt, copper, lead, mercury, selenium, silver, and zinc. Of 642 analyses, about 65 percent of the observed concentrations were zero. Only three samples contained metals in excess of U.S. Public Health Service recommended drinking water standards-two selenium concentrations and one cadmium concentration. A total of 213 samples were analyzed for 11 pesticidal compounds. Widespread but very low-level occurrence of pesticide residues in the "natural" environment was found-about 30 percent of all samples contained low-level concentrations of pesticidal compounds. The DDT family of pesticides occurred most commonly, accounting for 75 percent of the detected occurrences. The highest observed concentration of DDT was 0.06 microgram per litre, well below the recommended maximum permissible in drinking water. Nitrate concentrations in the "natural" environment generally varied from 0.2 to 0.5 milligram per litre. The average concentration of nitrate in many major streams is as much as 10 times greater.

The relationship between dissolved-solids concentration and discharge per unit area in the "natural" environment for the various physical divisions in the United States has been shown to be an applicable tool for approximating "natural" water quality. The relationship between dissolved-solids concentration and discharge per unit area is applicable in all the physical divisions of the United States, except the Central Lowland province of the Interior Plains, the Great Plains province of the Interior Plains and the Basin and Ridge province of the

Intermontane Plateaus. The relationship between dissolved solids concentration and discharge per unit area is least variable in the New England province and Blue Ridge province of the Appalachian Highlands. The dissolved-solids concentration versus discharge per unit area in the Central Lowland province of the Interior Plains is highly variable.

A sample collected from the hydrologic bench-mark station at Bear Den Creek near Mandaree, N. Dak., contained 3,420 milligrams per litre dissolved solids. This high concentration in the "natural" environment indicates that natural processes can be principal agents in modifying the environment and can cause degradation. Average annual runoff and rock type can be used as predictive tools to determine the maximum dissolved-solids concentration expected in the "natural" environment.

reference: Water Quality of Hydrologic Bench Marks-An Indicator of Water Quality in the Natural Environment, U.S. Geological Survey Circular 460-E by J.E. Biesecker and D.K. Leifeste.

Cooperative Programs

The cooperative programs of USGS with a variety of federal, state and local agencies generates a significant amount of water quality data of use to water-quality modelers. Many of these data result from short-term or synoptic data collection efforts. The data is published in annual State publications such as Water Resources Data for Texas Water Year 1977, Volume 1. Arkansas, Red, Sabine, Neches, Trinity River basins, and intervening Coastal basins, U.S. Geological Survey Water-Data Report TX-77-1, 585 p. The data are also available on computer data bases such as WATSTORE.

River Quality Assessments

In addition to the need to assess the effectiveness of pollution control efforts, there is a need to predict the effects of proposed management alternatives so that the best development plans can be selected. In its capacity as the appraiser of the Nation's mineral resources, the U.S. Geological Survey is developing and demonstrating techniques for making such predictions.

In this River-Quality Assessment research, teams of Survey scientists study all aspects of river quality in a drainage basin and determine the relative importance of river-quality problems, their causes, and the relative effectiveness of proposed solutions. The most efficient management actions can be determined from these studies to provide the best water quality at least cost. A series of these studies will be conducted by the Survey to demonstrate their usefulness and techniques for making them.

In a pilot assessment completed on the Willamette River in Oregon, the scientists analyzed several river-quality problems.

> Maintenance of high levels of dissolved oxygen in the river;
>
> Growth of algae as a potential nuisance;
>
> Occurrence and distribution of toxic trace metals; and,
>
> Potential for excessive soil erosion with increasing basin development.

The team found that waste-treatment plans already in effect had greatly reduced the input of oxygen-using wastes to the river and that dissolved-oxygen levels had improved greatly during recent years. Summer releases of freshwater from upstream reservoirs to aid river navigation had resulted in further improvements, which is an example of one management action serving two beneficial purposes.

Nevertheless, some additional improvement in the dissolved oxygen content was desirable to provide a greater margin of safety for the future. A very costly plan for advanced treatment of municipal wastes had been proposed as a possible solution. The results of the river-quality assessment showed, however, that elimination of a very few industrial discharges of ammonia wastes would result in greater improvement in the river at much less cost.

The releases of fresh reservoir water during low flows also have helped control the growth of undesirable algae in several ways:

> The freshwater provides a continuous low-level source of nutrients favorable to the growth of desirable algae.
>
> The increased flow quickly moves algae out of the river system.
>
> The released water is lower in temperature and in certain trace elements, which results in slower algal growth.

A study of trace metals in bottom sediments indicated no areas with concentrations high enough to cause immediate concern.

Population and industry are expected to increase greatly over the next 50 years in the Willamette Valley. To help evaluate the probable effects of such growth on land and water quality, a photomosaic map and an erosion potential index are used to estimate the way various land uses can affect soil erosion and sediment deposition in different types of terrain. These maps can be used by planners to make decisions on future land and water management within the river basin.

The major benefit of the Willamette River assessment is that it indicates that some proposed high cost pollution-control measures may be unnecessary; as a result the potential savings over the next 10 to 20 years could amount to tens of millions of dollars.

Additional assessments are now being carried out in the other river basins, e.g., Appalachicola River, Florida, Chattahoochee River, Georgia, Schuylkill River, Pennsylvania and the Carson-Truckee Rivers, Nevada. Because the combination of problems addressed in each basin is different, a variety of examples will be available to demonstrate the benefits of the river-quality assessment approach to those who must make river-quality management decisions.

reference: River Quality Assessment by Benjamin L. Jones,
U.S. Government Printing Office, 1977.

National Water Use Program

The National Water Use Program is a cooperative federal-state program designed to collect, store, and disseminate water use data to compliment data on availability and quality of the nation's water resources. Design of the program specifies measurement of a broad range of water use elements which were selected to meet many of the information requests of groups involved in planning, management, and operation on national, regional, and local levels. The primary objectives are (1) to account for the water used throughout the United States; (2) to organize the data collected so that it may be retrieved and used at the national, regional, and local levels; (3) to manage the program so that the data will be uniform in quality; and (4) to provide the necessary information to be able to update and make projections of future water requirements.

The nation's fresh and saline waters are under stress from increasing demands for water for domestic, industrial, agricultural, and other uses and from demands for greater protection of water quality. Competition for the available resources for diverse uses dictates that available supplies be matched with uses most beneficial to the common good. Relatively detailed information is being collected describing quantity and quality of water that is available, but relatively little information is available or is being collected describing quantities that are being used, where used, for what uses, and water quality changes that result from uses. Without adequate information on uses of water, decision-makers cannot, and have not, been able to resolve many critical water problems involving water-quality residuals, environmental impact, energy development, and resource allocations.

The National Water Use Program will provide for the storage of both detailed inventory data at the state level and aggregated estimates of water use at the national level (extrapolated from the state-level data). This data will be readily available to the local and Federal user communities to meet the following requirements:

A. Local

1. Determine present and projected water uses.
2. Quantify environmental pressure placed on water resources.
3. Support comprehensive water resource planning.
4. Minimize the impact that water resource availability has on the environment.
5. Minimize the economic expense of water resource planning.
6. Support conservation and preservation of water resources.
7. Permit intelligent participation in Federal planning.
8. Provide communication linkage among the agencies with the water resource community.

B. Federal

1. Provide for the optimum utilization of the nation's water resources.
2. Collect, store, and disseminate water-use data to complement data on availability and quality of the nation's water resources.
3. Provide an efficient, economical tool to support interbasin planning.
4. Support and enhance the data available to produce the "National Assessment" of the nation's water resources.
5. Provide a means of making more timely and accurate forecasts of water use throughout the nation.

Direction, management, and standards developed to provide for a national, consistent, and comprehensive program is the responsibility of the Survey. Manpower-intensive field activities for acquisition of the data will be the responsibility of the local agency, where direct communication with the water-using community can be readily established. How these responsibilities are implemented will ultimately reside with the State USGS District Chief and the cooperator.

The National Water Use Program will take a phased approach to implemetation. The software to support and maintain the data at the national level will be implemented during the first half of calendar year 1979. Additional national-level reporting, forecasting, and support software will be developed later as required by the U.S. Geological Survey.

The cooperative programs between the states and the Survey for the collection, storage, and dissemination of detailed state-level data were begun in fiscal year 1978 and will be fully implemented by 1982.

The responsibility for disseminating raw data collected at the state level rests with each state. In each state, an organization must be selected to provide a user liaison for this purpose.

At the national level, the USGS will provide a user liaison service for disseminating the aggregated data stored in the national data base.

Although both state and USGS personnel may be able to aid users in understanding the data stored by the Water Use Program, the final interpretation of water use data and projections made from that data are solely the responsibility of the individual user. The data will be indexed in the NAWDEX system.

Information about the water use program in each state may be obtained through the USGS District Chief in each state. Additionally, information about the program may be obtained from:

Fred Ruggles
U.S. Geological Survey
National Center
12201 Sunrise Valley Drive
Reston, Virginia 22091
Phone: (703) 860-6877

reference: The National Water Use Program Information Sheet, U.S. Geological Survey, 1978.

SEPARATION OF TIME-VARYING PARAMETERS IN STREAM WATER QUALITY MODELING

By

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Summary

In this study a set of equations were developed which can be used to separate the time-varying effects from observed DO data. It allows a reasonable stream simulation such that both the model and the data used in its formulation do not contain DO due to biological activities. Biological DO production and consumption are complex phenomena. By excluding these highly variable processes, this method simplifies stream DO modeling considerably. The net oxygen input due to this process exists only part of the day, but, in the stream waste assimilative capacity analysis and waste load allocation, one would focus his attention on critical conditions. Hence, unless the change of stream ecology is the main concern, it is desirable to formulate a stream water quality model without this time-varying term.

Discussion

In a stream containing phytoplankton biomass and benthic plants, the processes of photosynthesis and respiration constitute the major oxygen source and sink. Photosynthesis is the biological synthesis of organic compounds by chlorophyll-bearing plants in the presence of solar energy. A by-product of this process is oxygen. On the other hand, oxygen is consumed by living organisms as a process of their respiration. Therefore, for a biologically productive stream, observed dissolved oxygen (DO) content is the result of several dynamic processes including photosynthesis and respiration. In the formulation of a stream water quality model, an independent term has to be included to accommodate these in-stream DO sources and sinks, otherwise the model calibration and verification must be conducted in such a way that photosynthesis and respiration action is deliberately separated from the observed DO data.

The processes of photosynthesis and respiration are time dependent. In a steady state stream with constant waste loadings, these processes are the only causes of diurnal DO fluctuation. Ideally, a natural water body with significant biological oxygen production and consumption should be analyzed in terms of a time-varying model which makes stream DO a function of both time and space (O'Connor and DiToro, 1970). However, the application of a time-varying model in many water quality applications is constrained for lack of field data and due to the numerical complexities in its solution. Therefore, a steady state model is still the most popular tool in water quality analysis.

Photosynthesis and respiration actions were ignored in the traditional approach to steady state stream modeling (Streeter and Phelps, 1925). Obviously, this is inadequate for a biologically productive stream. In order to calibrate a model by this approach, it would be necessary to incorporate photosynthesis and respiration actions with other model parameters. As a result, the satisfactory hydraulic and bio-chemical simulation for a stream can hardly be achieved.

More recently, an average net daily photosynthesis and respiration rate has been added in steady state stream modeling. The model calibration and verification are conducted based on average DO (e.g. Zitta, et al, 1977). This approach also has its limitations. First, the rate of net biological oxygen production is often difficult to evaluate due to the lack of a thorough understanding of the biological activities in a stream (Rutherford, 1977). Thus, estimates of net stream photosynthesis and respiration rate based on data from a particular survey and its use in model projection is unreliable. Secondly, because of the supersaturated DO condition during daylight hours, average DO in many streams is high while DO content may be significantly below the stream standard for the rest of the day. From a water quality management standpoint, therefore, the average DO is not a good index.

In the Study now reported, a new method was developed which separates the time-varying effect from observed DO data before using them in model calibration. As a result, both the stream water quality model and the DO data used in its calibration and verification are completely in the steady state mode. This leads to a reasonable model formulation in the sense that the evaluated model parameters represent the true hydraulic and biochemical behavior in a stream. This concept was initially proposed by Lawler, Matusky & Skelly Engineers in their Susquehanna River Study (1975), and was called a "Scrubbing" method. However, the "Scrubbing" technique consists of the determination of net photosynthesis rates before the modification of observed DO data. It thus requires a series of tedious computations. Furthermore, in the mathematical formulation of "Scrubbing" technique, convective changes of DO was dropped as insignificant to the diurnal variation, which in many instances, may not be wholly justified.

With this in mind, a new mathematical formulation for diurnal stream DO variation was conducted in this study and a set of new formula derived which allows the separation of photosynthesis and respiration actions from observed DO, based only on observed DO data and stream hydraulic characteristics.

Mathematical Formulation

In fluid dynamics, there are two methods of describing the motion of a group of particles in a continuum, i.e. the Lagrangian method or the Eulerian method. In the Lagrangian representation a particle in the flow field is chosen arbitrarily at some time and the motion of the fluid is given by the subsequent motion of this particle. Alternatively, the changes in velocity at an arbitrarily chosen position as time elapses are studied in the Eulerian method. (Daily and Harleman, 1966). Eulerian representation was found to be more convenient in the investigation of diurnal variation at any stream point, and is adopted in this study.

Using the Eulerian method, flow properties at any particular point in the flow field can be expressed in terms of a total or substantial derivative. In a one dimensional stream, dissolved oxygen content in the vicinity of a stream point is:

$$\frac{dD}{dt} = \frac{\partial D}{\partial t} + U \frac{\partial d}{\partial s} \qquad (1)$$

The first term on the right hand side of the equation (1) represents the "local" change as a function of time and the second term is the "convective" change dependent on the motion of the field particle in a stream. Here D is DO deficit, in mg/l, or the difference of saturation concentration of DO and the actual concentration. U is the mean velocity at that stream point, in mile/hr. Of the two independent variables, t refers to the time of diurnal variation, in hrs., and s is the distance along the path of flow particles, in miles.

Water quality models are often used in the study of a critical water quality conditions when low flow and high temperature are prevalent. Therefore, the stream flow can be reasonably assumed to be steady and uniform, and "local" changes consist of only the action of photosynthesis and respiration. In a polluted stream, "convective" change of DO is the result of organic waste decay and atmospheric reaeration. Hence, the substantial derivative of DO at a stream point becomes:

$$\frac{dD}{dt} = R - P(t) + K_1 L - K_2 D \qquad (2)$$

Here P and R are the rates of photosynthesis and respiration, in mg/l/hr. Note that P is a function of time, while the rate of plant respiration can be assumed a constant (Odum, 1956). K_1 and K_2 are the rate of biochemical oxidation of organic wastes, or deoxygenation coefficient and the rate of stream reaeration, in 1/hr., respectively. For the sake of simplicity, a single term L is used in equation (2) for both carbonaceous and nitrogenous biochemical oxygen demanding materials (BOD).

In a typical diurnal DO fluctuation, two equilibrium points exist (Figure 1). At nighttime equilibrium, when DO deficit is a maximum D_r, equation (2) is:

$$\frac{dD}{dt} = R + K_1L - K_2D_r = 0 \tag{3}$$

Similarly, at daytime equilibrium, when DO deficit is at its minimum D_p, equation (2) is:

$$\frac{dD}{dt} = R - P_{opt} + K_1L - K_2D_p = 0 \tag{4}$$

Here P_{opt} is the optimal rate of photosynthesis. Early studies indicated that for the phytoplankton biomass and benthic plants in a natural water body the rate of plant respiration is relatively constant and amount to about 10% of the optimal rate of photosynthesis (Ruttner, 1963 and Odum, 1952). Or,

$$R = 0.1\ P_{opt} \tag{5}$$

D_w is the stream DO when photosynthesis and respiration actions are not presented. Therefore, at the vicinity of D_w, equation (2) takes the form of:

$$\frac{dD}{dt} = K_1L - K_2D_w = U\ \frac{dD_w}{ds} \tag{6}$$

Here $U\ dD_w/ds$ replaces the partial derivative $U\ \partial D/\partial s$ of equation (1) since without photosynthesis and respiration action, stream DO is a function of distance alone. Solving equations (3), (4), (5) and (6) simultaneously, one would have:

$$D_w = D_r - 0.1\ (D_r - D_p) - S_s/K_2 \tag{7}$$

Here D_r and D_p can be directly read on the diurnal curve. $S_s = U\ dD_w/ds$ can be derived by multiplying the slope of the observed stream DO profile and average stream velocity. DO profile of minimum observed DO may be used, because the difference between minimum DO and D_w is respiration R, which is relatively constant.

K_2 is stream reaeration which can be determined based on simple hydraulic data (Rathbun, 1977).

During the daylight hours, supersaturated DO may exist in a stream, or DO deficit D_p becomes negative. Following the above procedure, D_w can be readily derived to be the following:

$$D_w = D_r - 0.1\ (D_r + D_p) - S_s/K_2 \qquad (8)$$

Equations (7) and (8) establish the required relationship whereby a stream's theoretical DO in the absence of photosynthesis and respiration can be determined based on observed DO data and stream hydraulic characteristics.

Application

An intensive stream water quality survey was conducted during the week of June 13-17, 1977 by the New York State Department of Environmental Conservation on Eighteen Mile Creek, which is located in Niagara County in northwestern New York. Survey data shows significant diurnal DO fluctuations in the Creek, especially downstream from Rt. 104 Bridge (Figure 1). Circles in Figure 1 are stream DO at each sampling station after the separation of photosynthesis and respiration actions. They were derived based on equation (7).

Eighteen Mile Creek was simulated in terms of a steady state one dimensional SNSIM model developed by EPA Region II (Braster, et al, 1975). Model parameters such as deoxygenation rate and stream reaeration were estimated on the basis of field data, and then modified during the model calibration. Details have been included in a New York State Department of Environmental Conservation Survey and Analysis Report (Liu, 1978). Figure (2) gives a computer plot of the model output. Comparisons of predicted and observed DO show good agreement and suggest a reasonable simulation of the Creek's hydraulic and biochemical behavior.

Acknowledgment

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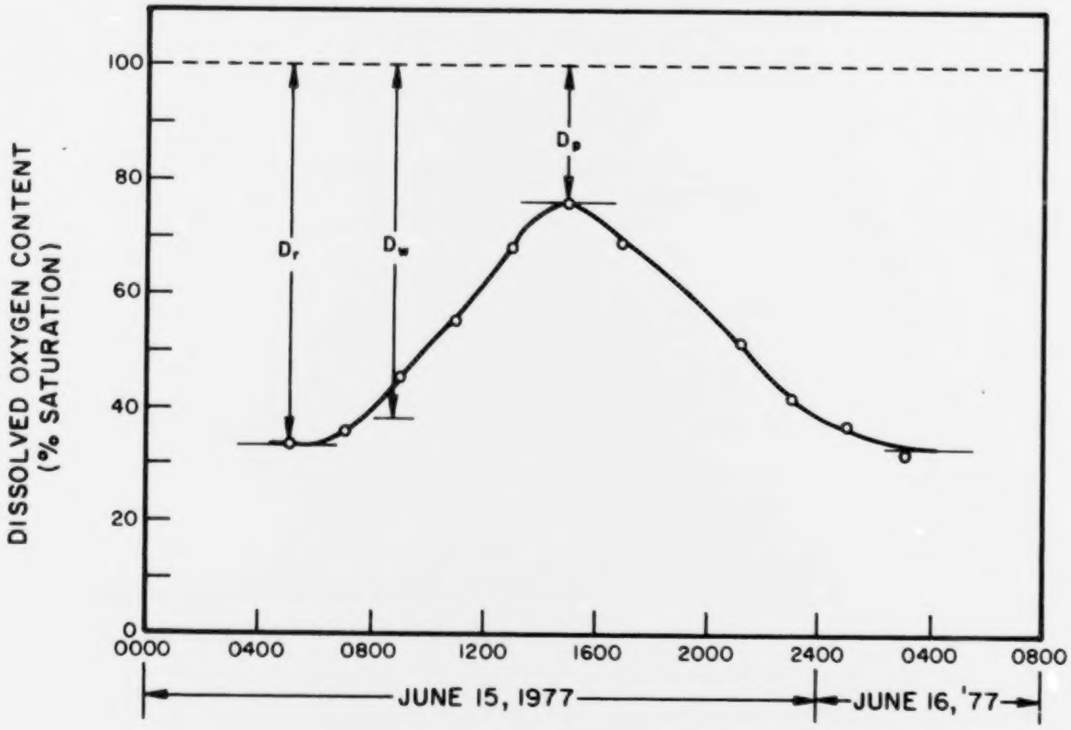

FIGURE 1. OBSERVED DIURNAL
DISSOLVED OXYGEN CURVE IN EIGHTEEN MILE CREEK

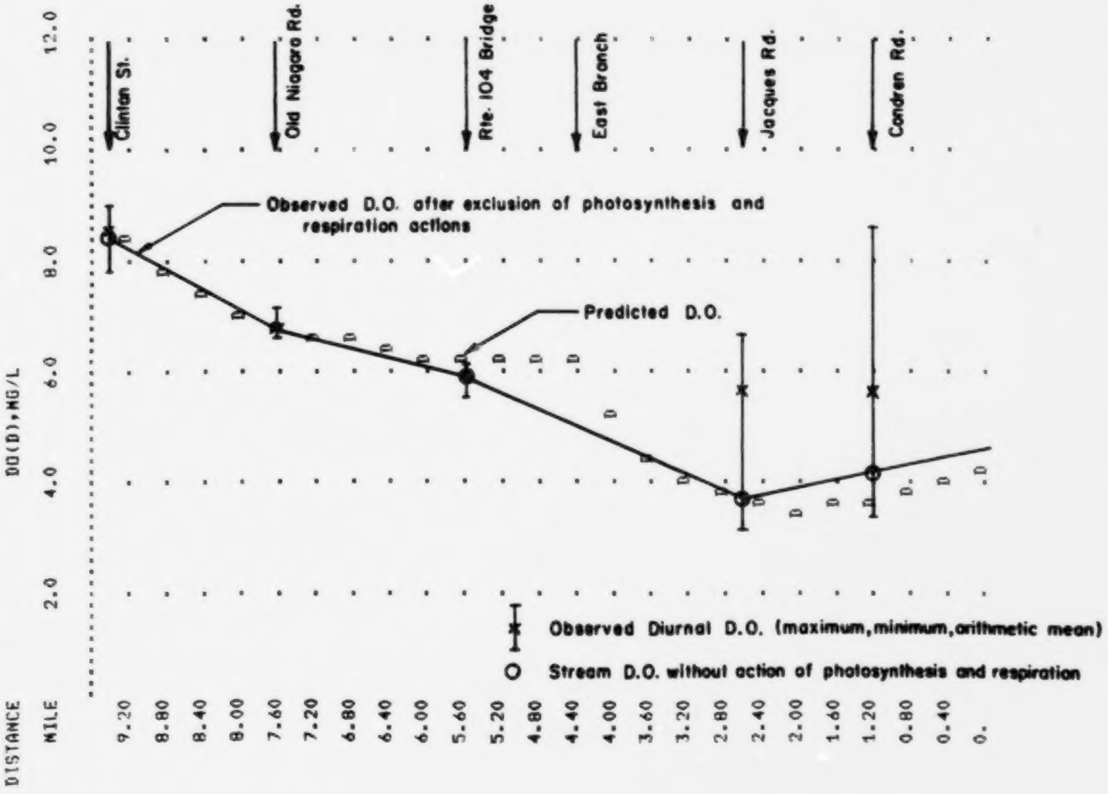

FIGURE 2 D.O. PROFILE AND MODEL PREDICTION, EIGHTEEN MILE CREEK, N.Y.

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EVALUATION OF HAZARDOUS SUBSTANCES TRANSPORT MODELING IN SURFACE WATERS

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Introduction

The environmental impact of various hazardous substances (e.g., pesticides, heavy metals, radionuclides, etc.) is an increasingly important issue (1,2,3). Although considerable effort is being made to minimize the release of these hazardous substances to the environment, decision makers must have a sound basis for impact assessment.

Mathematical models supported by well-planned data collection programs can be useful tools in assessing migration and ultimate fate of hazardous substances in surface waters. In order to obtain accurate predictions of contaminant transport, mathematical models must include major transport mechanisms. These mechanisms include:

1. advection and diffusion/dispersion of hazardous substances
2. chemical and biological degradation and decay due to hydrolysis, oxidation, photolysis, volatilization, and biological activites
3. parent-daughter products of radioactivity decay
4. contribution of hazardous substances from outside sources into the system
5. interaction between sediment and hazardous substances, such as contaminant adsorption by sediment; contaminants desorption from sediment to water; transport of particulate contaminants (those associated with sediment); deposition of particulate contaminants to the bed; and resuspension of particulate contaminants from the bed.

Until recently sediment-contaminant interaction was not included in models because of the complex nature of sediment transport and the contaminant adsorption/desorption mechanisms (4,5). However, significant effects of sediment-contaminant interaction on the transport of hazardous substances are well documented. For example, field measurements conducted in the Clinch River, Tennessee, indicated that approximately 90% of the radionuclide, cesium-137, released from the Oak Ridge National Laboratory was adsorbed by the suspended sediments in the river within 35 km downstream of the effluent discharge (6). In another study the majority of Kepone, a pesticide released to the James River Estuary, Virginia, was also judged to be associated with sediment (1).

Transport Models

Most of the mathematical models for the transport of hazardous substances are based on the general advection-diffusion equation. These models range from simple analytical solutions to complex numerical models. Because of severe limitations imposed on analytical solutions, applicability of these solutions is very limited. Instead, numerical models must be used to accommodate wide variations of channel geometry, flow characteristics, and characteristics of sediment and hazardous substances in most study areas.

Most water quality models that can be used to simulate the transport of hazardous substances in surface waters include only the mechanisms of advection and diffusion/dispersion, degradation and decay, parent-daughter product of radioactivity decay, and contributions from outside sources (4,7). These models are applicable to short-term migration cases where: 1) the contaminant has a very small distribution coefficient, Kd, and 2) sediment concentration is very low.

However, in cases where: 1) the Kd is very large; 2) sediment concentration is high; or 3) long-term migration is concerned, mathematical models must include sediment-contaminant interaction by coupling sediment and contaminant transport modeling (2,8-12). Sediment-contaminant interaction becomes very important because under one or more of these conditions, a significant amount of hazardous substances in surface waters is adsorbed from solution onto sediment. Thus, otherwise dilute contaminants are concentrated. This process may create a significant pathway to man. Contaminanted sediments may be deposited into river and ocean beds, becoming a long-term source of pollution through desorption and resuspension. In contrast, sorption by sediment can be an important mechanism for reducing the area of influence of these hazardous substances by reducing dissolved concentration of hazardous materials. Moreover, since the movements and adsorption capacities of sediments vary significantly with sediment size fractions, transport of sediment and particulate contaminants must be simulated for each sediment size fraction. Mathematical models which do not include these sediment-contaminant interactions may produce errors in predicting the migration of hazardous substances.

As revealed by a recent study (13), very few models are capable of solving the transport of hazardous substances by including sediment-contaminant interations (2,8-12). In order to fully accommodate sediment-contaminant transport, mathematical models must couple:

- sediment transport for each sediment size fraction
- dissolved contaminant transport
- particulate contaminant transport for each sediment size fraction
- bed history of sediment and contaminant.

Currently the following three models include these four components:

1. CHNSED, developed by Field et al., (12) is an unsteady, one-dimensional model applicable to rivers. It was applied to the Rio Grande River (New Mexico).

2. SERATRA, developed by Onishi et al., (9) is an unsteady, two-dimensional (longitudinal and vertical) model applicable to rivers and lakes. SERATRA has been applied to the Columbia River (Washington), Clinch River (Tennessee), Four Mile and Wolf Creeks (Iowa) and Cattaraugus and Buttermilk Creeks (New York).

3. FETRA, also developed by Onishi et al., (2,14) is an unsteady, two-dimensional (longitudinal and lateral) model applicable to rivers, estuaries and oceans. This model was applied to the James River estuary (Virginia).

Data Requirement

One of the most important aspects of mathematical modeling is the required field data. For transport modeling the required data are:

1. channel characteristics
    - cross-sectional shapes (or bathymetry)
    - plan geometry
2. fluid characteristics
    - viscosity
3. flow characteristics
    - distribution of depth
    - distribution of velocity

- wave characteristics in oceans and large lakes
- salinity
- temperature
- diffusion/dispersion coefficient

4. sediment characteristics

   - diameter, density, and minerology of sediment
   - critical shear stresses of sediment (or other sediment transport parameters)

5. characteristics of hazardous substances

   - adsorption/desorption rates (or distribution coefficients)
   - chemical and biological degradation or decay rates

Accuracy of model prediction is significantly affected by the integrity of data used for the modeling. However, because of the cost and time involved, field sampling activities have been rather limited. Furthermore, for most instances, field sampling programs and computer simulation programs have not been coordinated. To make the best use of cost and time, as well as provide accuracy of the prediction, field sampling planners and mathematical modelers must coordinate their investigations very closely.

The amount of data required is basically proportional to the sophistication of the models. However, simpler models require more judgmental data than more sophisticated models. For example, a steady, one-dimensional model requires very careful selection of the longitudinal dispersion coefficient when it is applied to an estuary. However, dispersion coefficients are less important when an unsteady, two- or three-dimensional model is applied.

Data are currently incomplete to accurately express the mechanisms of degradation and decay, and sediment-contaminant interaction. (Among these data, those describing the sediment-contaminant interaction, especially adsorption/desorption mechanisms and migration of cohesive sediment, are most urgently needed because of their significant effects on the movement of hazardous substances.) For example, a functional relationship of the distribution coefficient with various sizes and types of sediments, organic content, and other water quality parameters must be established to more accurately describe adsorption/desorption mechanisms. The time variation of Kd must also be determined. Because of these incomplete data and parameters to express these important mechanisms, extensive efforts must be exercised to conduct comprehensive field and experimental data collection.

Verification

Mathematical models must be calibrated and verified under a wide range of conditions, prior to the application of the model, to produce accurate and more defensible prediction of transport phenomena. Currently only a few models are at least partially verified against field data (2,5,7,9). There is a definite need to obtain detailed field data and to verify models with these data. Verification of existing models is probably more important than creating a new unverified model.

Recommendations

When evaluating the transport of hazardous substances in surface water, the following steps are recommended:

1. Examine available models to identify general applicability and limitations of models.

2. Select potential simulation models for transport of hazardous substances in rivers, estuaries, oceans and impoundments for further detailed verification tests.

3. Perform literature search for available field data and/or perform coordinated field data collection, laboratory physical modeling and laboratory experiments to obtain data needed for model verification.

4. Perform model verification tests with these measured data to examine selected models.

5. Select most suitable models identified for rivers, estuaries, oceans and impoundments.

6. If none of the models are appropriate, modify the models most suitable for the specific application, and then verify those models.

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THE USE AND VERIFICATION OF HYDRODYNAMIC MODELS IN WATER QUALITY MODELS

By

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The real usefulness of hydrodynamic models is in their application in water quality models. It is the hydrodynamic transport which transports material through the nearshore region into the main part of the lake and which mixes material that is already present in the lake. The significance of the hydrodynamic transport in a particular water quality application depends on the actual problem investigated: the hydrodynamic transport is unimportant for a lake treated as a completely mixed reactor while it can be extremely important for a lake divided into many segments. This comparison points out that the real distinction for many water quality problems is in the scales that are involved, i.e., the time and length scales that the important mechanisms are assumed to occur over and that have to be included in the model. Difficulties arise because hydrodynamic models have been traditionally calculated over relative ly small time and length scales (on the order of minutes and kilometers), and water quality models have been traditionally calculated on relatively large time and length scales (on the order of seasons of the year and hundreds of kilometers). It has not been unusual for water quality modelers to state that it is impossible to use hydrodynamic models because of the exorbitant computer costs and because of the difficulty in extracting the meaningful information that the water quality models need. Similarly, the hydrodynamic modelers have stated that it would be a meaningless exercise to try and use their models in the water quality models because these models have such crude time and length scales. The real problem comes down to how the models with fine time and length scales can be used in conjunction with models that have much larger time and length scales. The solution to this is not to just average the small scale calculations to arrive at some larger scale motion. This approach completely eliminates the smaller scale motion that contributes to what is called the mixing in the larger scale models. What has to be done is to properly account for this small mixing in the larger scale model. The method that is being employed at the Large Lakes Research Station (LLRS) is similar to the Reynolds partitioning idea used to derive the turbulence equations. (Quantities are written as some mean value and a fluctuating component about that mean. These expressions are used to derive equations for the mean quantities). In our method we consider the small scale quantities as a mean value over the larger scales and as a fluctuating component about that mean. Equations can then be derived for the large scale quantities which account for the small scale mixing. This appears to be the proper way to deal with the change in scales.

If we say that the major use of the hydrodynamic models will be in their application in water quality models, then we should say that the hydrodynamic models be verified on the same time and length scales as the water quality models. What kind of confidence can one have in the use of a model if it is verified against data for a couple of hours or days and then used for an application that extends for a year or more? The only way you can verify a hydrodynamic model this way is to calculate the transport of some material in the water for the whole period of time you are interested in. This does require a lot of data to compare with. One way to satisfy this requirement for data is to employ remotely sensed data. For example, the Nimbus 7 satellite is presently in orbit and provides coverage 5 out of every 6 days with a resolution of 800 meters. The hydrodynamic model could be used in conjunction with a transport model for suspended solids in the water and compared with the satellite data. Ship cruises would also have to be employed to provide ground truth and give some vertical distribution in the water. A lot more data would be available this way than if just shop cruises were employed. Some of the models at LLRS are presently being verified with data obtained by remote sensing and by ship cruises.

TOXIC SUBSTANCE MODELING RESEARCH AT THE LARGE LAKES RESEARCH STATION

By

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Introduction

The U.S. Environmental Protection Agency (EPA) is confronted with an enigmatic responsibility of managing environmental quality. The key question that ultimately arises during the course of its job is: What quantity of a substance, if any, can be allowed to be discharged and yet maintain the quality and associated uses of the system? In fact, this is the primary task confronting EPA in the implementation of the Toxic Substance Control Act (TSCA) - to regulate or control the discharge of substances or mixtures which "...present an unreasonable risk of injury to health or to the environment..."

Regulation of toxic substances will not be done, however, without consideration of industrial and market concerns. Thus one of the principles recognized by Congress in preparing this legislation is that a risk free society is not obtainable (1). Also, as stated by William Butler, General Counsel, Environmental Defense Fund:

> "Environmentalists wish to see established some rational method of toxic chemical control which will maximize benefits of chemicals while at the same time minimize their unintended hazards to human health and the environment.

Although, as Mr. Butler continues,

> "Let's not kid ourselves, we have a long way to go before achieving that goal."

As a result of these viewpoints which reflect technilogic, economic and social realities, we will always be confronted with certain amounts of marginally hazardous substances in the ecosystem.

The modeler's goal is and has been to provide at least some rational input to the regulatory process whatever the environmental issue. The modeling-management process can be depicted by the flow chart shown in Figure 1. The process consists of four primary areas: 1) information gathering, 2) modeling, 3) health effect assessment, and 4) decision making. Information gathering includes:

1. Quantification of existing or expected discharges or emissions.
2. Measurements of ambient concentrations in various compartments of the ecosystem.
3. Experimentation to obtain process routes and rates.

Modeling can involve two separate types: 1) diagnostic and, 2) prognostic. Diagnostic modeling includes the synthesis of surveillance and experimental data into a calculation that is able to emulate the real world. If this is done satisfactorily then the model might be used for prognostic analyses, i.e., simulations of biochemical concentrations (dose) in space and time. These prognostics may be used for regulatory purposes along with health effects data (allowable doses) to decide what amount, if any, can be allowed into the ecosystem.

A strategy for Toxic Substance Modeling research has been formulated for the Great Lakes by Wayland Swain (3), as shown in Figure 2. This might be referred to as an ecosystem approach. The unique aspect is that it proposes to quantify the sources, reservoirs, exposure routes, dose levels and health effects of chosen chemicals for selected geographical areas. It would provide the necessary data for a complete diagnostic evaluation.

This approach has been initiated in part for Saginaw Bay, Lake Huron. Samples have been collected starting in 1977 and are being analyzed for PCB. Initially the data will be used to perform a materials balance to see if PCB can be accounted for in all compartments. Then this will be expanded to include adsorption-desorption, and biological processes. Because of the complexity and expense of laboratory start-up only some of the water compartment data are available for 1977.

The results of this preliminary materials balance are shown here for exemplary purpose only. The results are preliminary and should not be used for citation since the values may change as more data become available. The purpose is to show the procedures followed in performing a mass balance. These include:

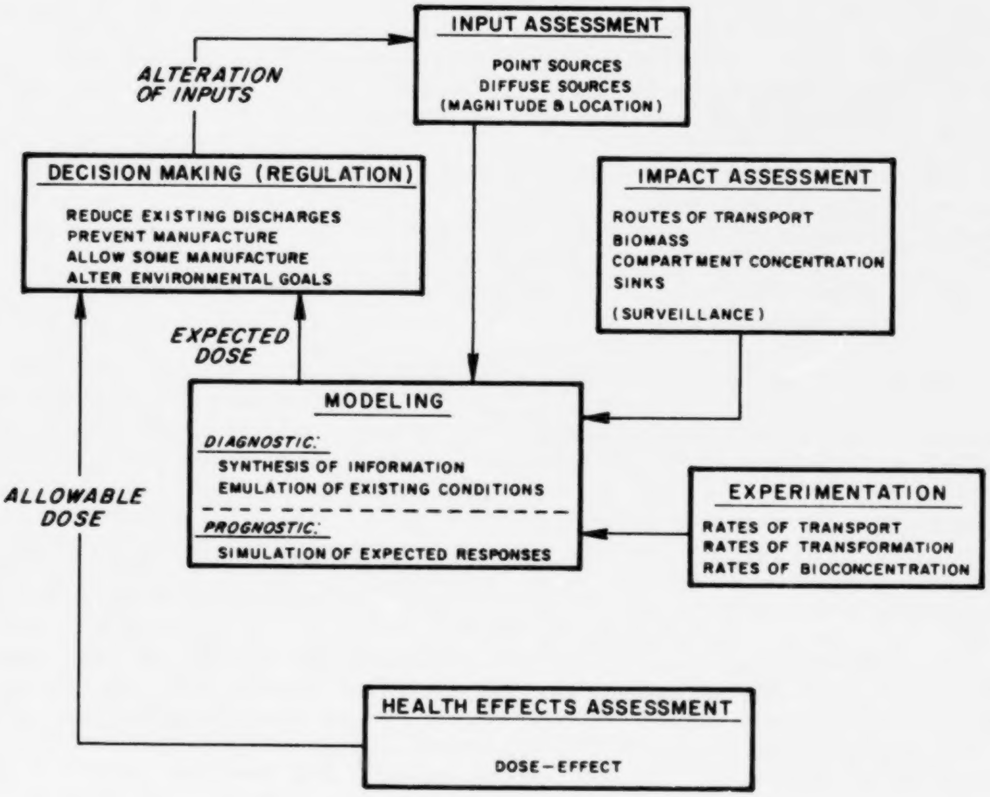

INPUT ASSESSMENT
POINT SOURCES
DIFFUSE SOURCES
(MAGNITUDE & LOCATION)
ALTERATION OF INPUTS
DECISION MAKING (REGULATION)
REDUCE EXISTING DISCHARGES
PREVENT MANUFACTURE
ALLOW SOME MANUFACTURE
ALTER ENVIRONMENTAL GOALS
IMPACT ASSESSMENT
ROUTES OF TRANSPORT
BIOMASS
COMPARTMENT CONCENTRATION
SINKS
(SURVEILLANCE)
EXPECTED DOSE
MODELING
DIAGNOSTIC:
SYNTHESIS OF INFORMATION
EMULATION OF EXISTING CONDITIONS
PROGNOSTIC:
SIMULATION OF EXPECTED RESPONSES
ALLOWABLE DOSE
EXPERIMENTATION
RATES OF TRANSPORT
RATES OF TRANSFORMATION
RATES OF BIOCONCENTRATION
HEALTH EFFECTS ASSESSMENT
DOSE-EFFECT

FIGURE 1. ENVIRONMENTAL MODELING-MANAGEMENT PROCESS

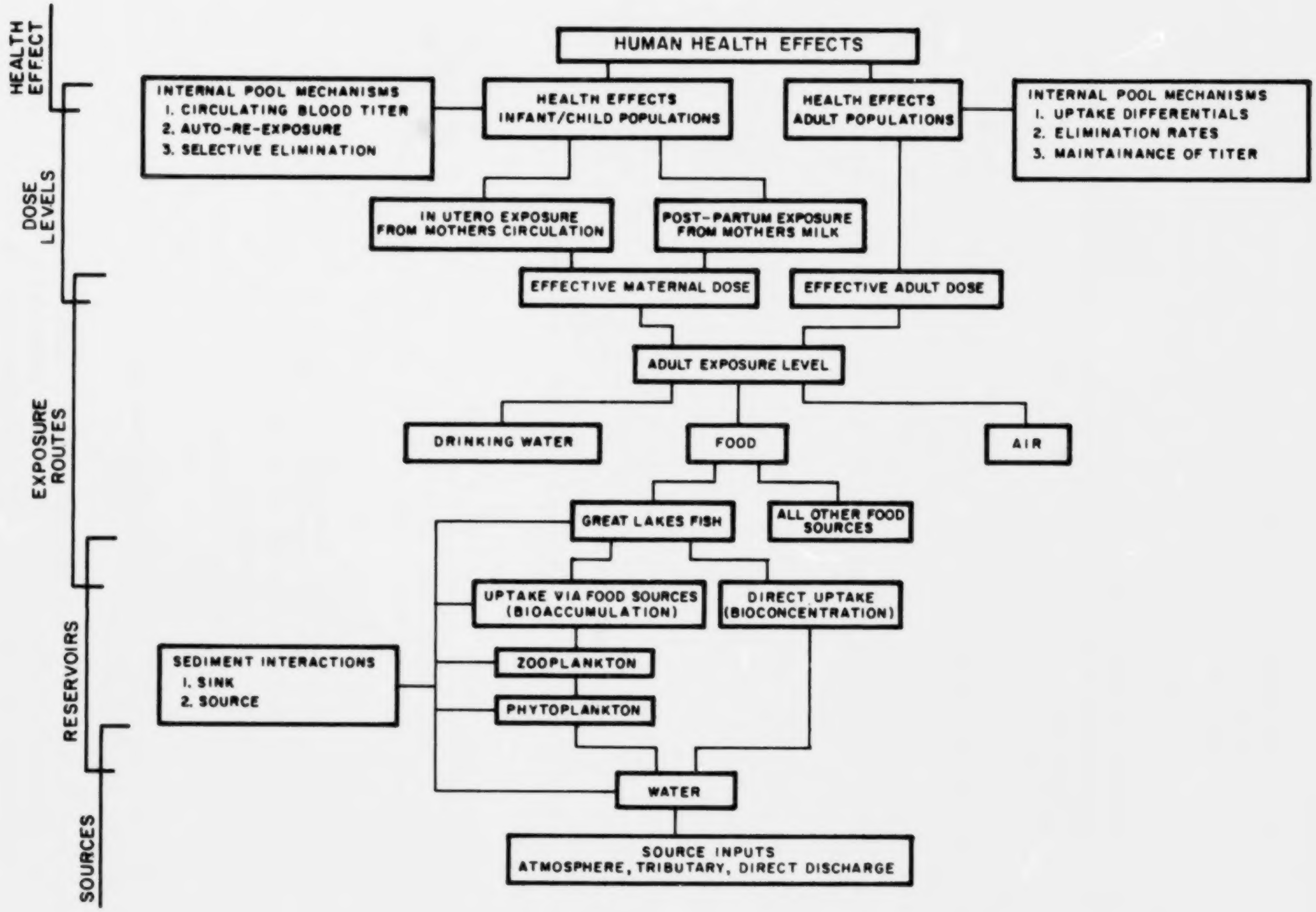

HEALTH EFFECT
DOSE LEVELS
EXPOSURE ROUTES
RESERVOIRS
SOURCES
HUMAN HEALTH EFFECTS
INTERNAL POOL MECHANISMS
1. CIRCULATING BLOOD TITER
2. AUTO-RE-EXPOSURE
3. SELECTIVE ELIMINATION
HEALTH EFFECTS INFANT/CHILD POPULATIONS
HEALTH EFFECTS ADULT POPULATIONS
INTERNAL POOL MECHANISMS
1. UPTAKE DIFFERENTIALS
2. ELIMINATION RATES
3. MAINTAINANCE OF TITER
IN UTERO EXPOSURE FROM MOTHERS CIRCULATION
POST-PARTUM EXPOSURE FROM MOTHERS MILK
EFFECTIVE MATERNAL DOSE
EFFECTIVE ADULT DOSE
ADULT EXPOSURE LEVEL
DRINKING WATER
FOOD
AIR
GREAT LAKES FISH
ALL OTHER FOOD SOURCES
UPTAKE VIA FOOD SOURCES (BIOACCUMULATION)
DIRECT UPTAKE (BIOCONCENTRATION)
SEDIMENT INTERACTIONS
1. SINK
2. SOURCE
ZOOPLANKTON
PHYTOPLANKTON
WATER
SOURCE INPUTS
ATMOSPHERE, TRIBUTARY, DIRECT DISCHARGE

FIGURE 2. A STRATEGY FOR TOXIC SUBSTANCE MODELING

W. SWAIN, LLRS, FEB.1979

1. Quantifying the transport structures of the Bay.
    a. estimate loadings for a trace substance, chloride
    b. trace this substance through the system in space and time, adjusting the transport coefficients until the calculated concentrations are equal to the measured (see Figures 5-8)
2. Estimate PCB loads (Figure 9).
3. Calculate expected PCB concentrations in each special compartment (Figures 10 and 11).
4. Evaluate results.

Figure 3 shows the sampling scheme and the priority stations at which this initial data are available. Figure 4 shows the location of the Saginaw River sampling location where samples are obtained to estimate loadings. As can be seen in Figure 7, the chloride data is well duplicated by the mass balance model, thus confirming the transport structure used for the PCB calculations.

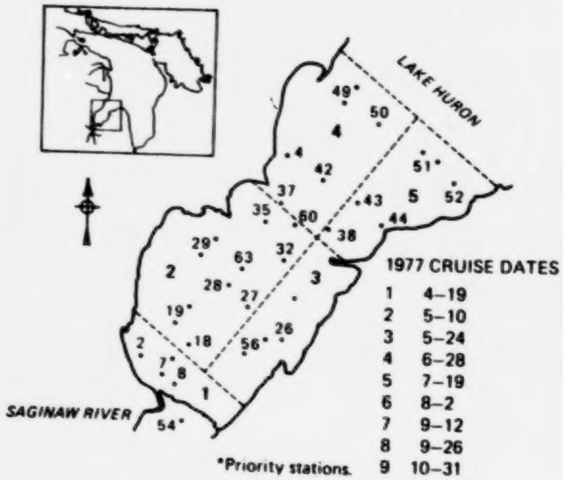
The estimated monthly PCB loads are shown in Figure 7 for mixtures Aroclor 1254 and 1016. Although 1016 loading is 2 to 3 times greater than 1254, 1016 was found in the bay above detectable levels too infrequently to do a mass balance; therefore, the mass balance was carried out for 1254 only. These results are shown in Figure 8 where calculated Aroclor 1254 concentrations are superimposed on the measured for each segment and over time. Although it is readily apparent that the simple mass balance model cannot adequately describe the data, the analysis does provide an initial insight into PCB transport in Saginaw Bay.

For example, when loadings are set equal to zero, the calculated concentrations seem to follow the lowest data points. This suggests that transient processes are occurring in the bay like rapid settling and resuspension of solids to which PCB are adsorbed.

The calculated mass of Aroclor 1254 in the entire bay is plotted in Figure 9. Over the data period of April through November, an average of 554 kg resided in the bay compared to 300 kg accounted for by the model. This suggests either an unknown source or a lack of sufficient data to describe the variability adequately. Obviously, more research is required.

However, several general conclusions can be drawn from this initial investigation.

1. If toxic substances are to be modeled in complex systems as Saginaw Bay, much expensive data are necessary for model calibration and verification.


LAKE HURON
SAGINAW RIVER
49* 50 4 .4 42 51* 5 52 37 35 60 .43 44 38 29* 63 32 2 28* 27 3 19* 26 .18 56* 2 7* 8 1 54*
*Priority stations.

1977 CRUISE DATES	
1	4–19
2	5–10
3	5–24
4	6–28
5	7–19
6	8–2
7	9–12
8	9–26
9	10–31

FIGURE 3. SAGINAW BAY 1977
SAMPLING NETWORK AND SEGMENTATION

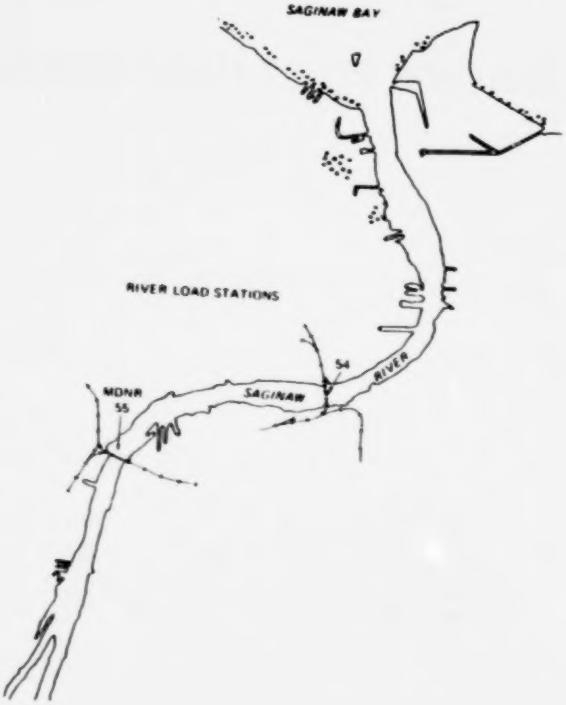

SAGINAW BAY
RIVER LOAD STATIONS
MDNR
55
54
SAGINAW
RIVER

FIGURE 4. SAGINAW RIVER 1977
SAMPLING NETWORK AND SEGMENTATION

PRELIMINARY INFORMATION, NOT FOR CITATION

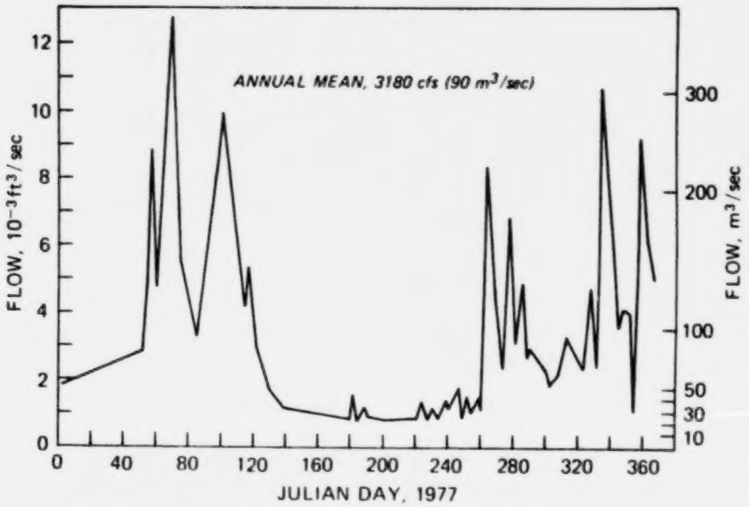


FIGURE 5. SAGINAW RIVER DAILY HYDROGRAPH, 1977

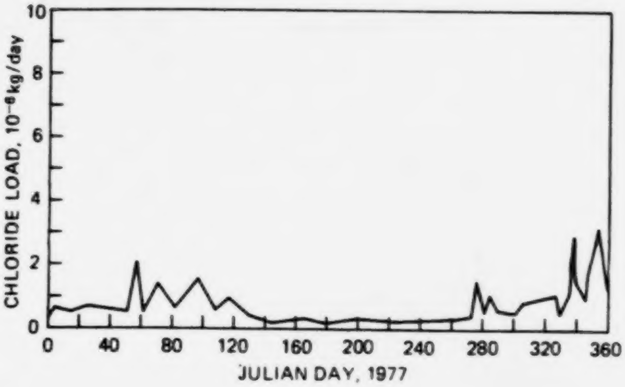


FIGURE 6. SAGINAW RIVER CHLORIDE LOAD, 1977

PRELIMINARY INFORMATION, NOT FOR CITATION

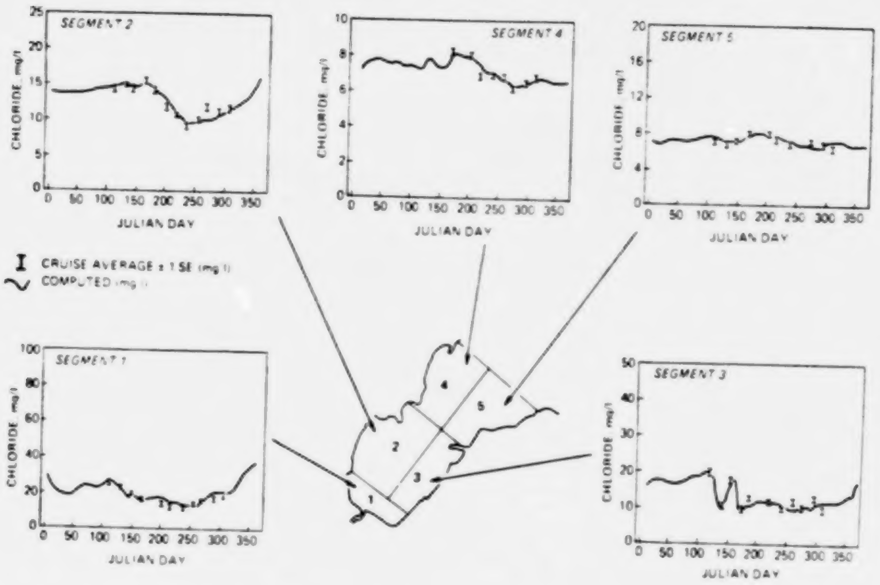


FIGURE 7. SAGINAW RIVER
CHLORIDE TOTAL SYSTEM, 1977

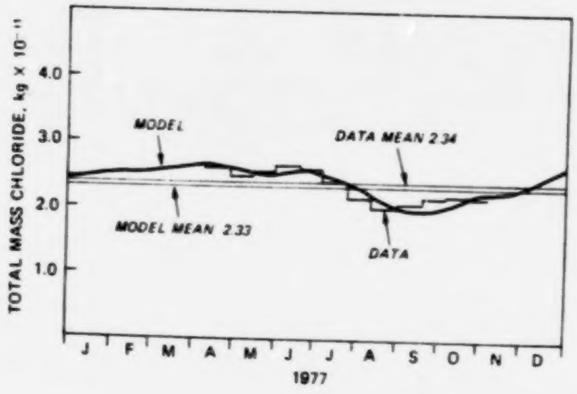
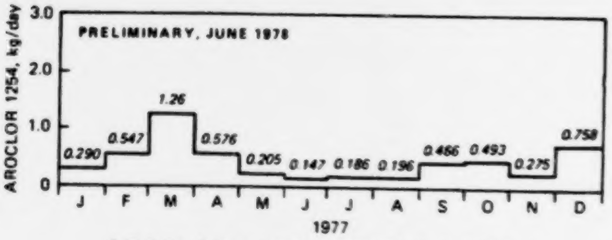
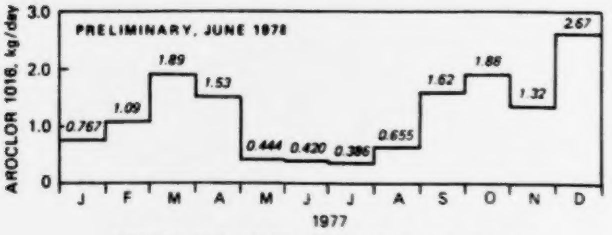


FIGURE 8. SAGINAW BAY
CHLORIDE TOTAL SYSTEM MASS, 1977

PRELIMINARY INFORMATION, NOT FOR CITATION



AROCLOR 1254 MONTHLY LOAD



AROCLOR 1016 MONTHLY LOAD

FIGURE 9. ŠAGINAW RIVER 1977 PCB DATA

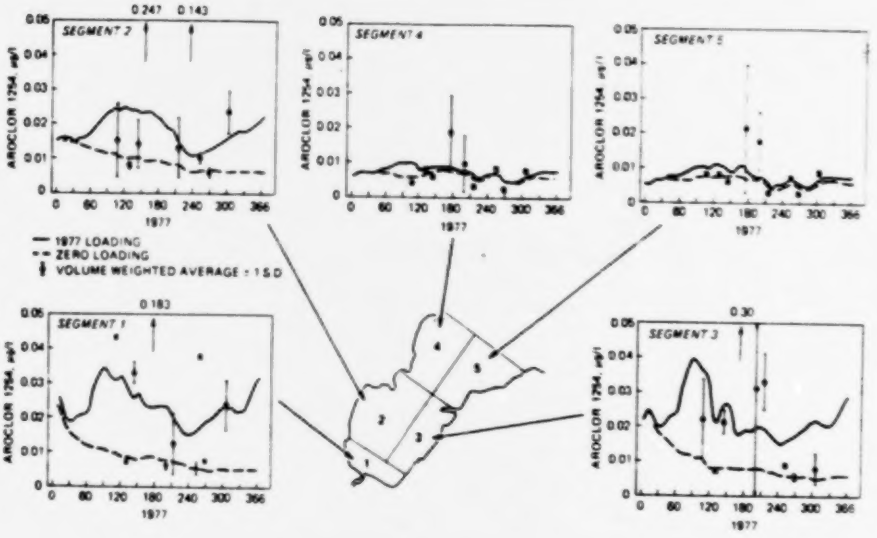


FIGURE 10. SAGINAW BAY AROCLOR 1254, 1977

PRELIMINARY INFORMATION, NOT FOR CITATION

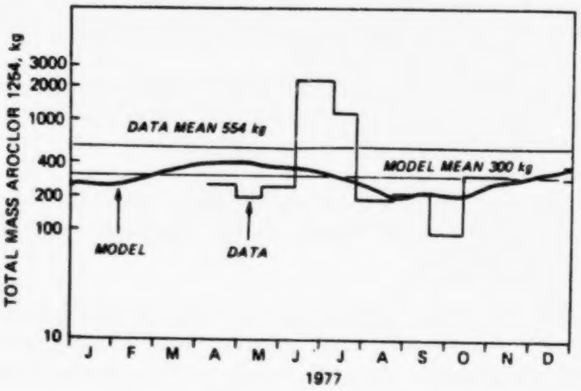


FIGURE II. SAGINAW BAY
AROCLOR 1254 TOTAL SYSTEM MASS

PRELIMINARY INFORMATION, NOT FOR CITATION

2. Toxic substance models are an extension of existing models which provide the foundation. These include physical transport models and nutrient-biomass models.

3. Therefore, surveillance for model development must continue to include traditional parameters and add on necessary toxic data. For example, we will always need data for input flows, conservative tracers, biomass at several levels of the food chain, nutrients for biomass growth, sediment interaction, temperature, and other physical parameters.

4. Models may provide the expected dose concentrations in space and time but will not provide effects.

5. Adequate computer resources and data bases must be available to the modeler if models are to be used in the decision making process.

6. Modelers must understand how the data were collected and analyzed and must help design the field programs and data bases.

7. Because of the expense of this holistic approach, a few well planned and executed integrated studies for a few selected substances are preferred over a diluted collection of data.

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(3) Swain, Wayland, Director, EPA, Large Lakes Research Station. Personal Communication. February 1979.

THE NEED FOR INNOVATIVE VERIFICATION OF EUTROPHICATION MODELS*

By

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Introduction

In recent years there has been a trend toward using more mechanistic models of the eutrophication process. By mechanistic, I mean models that account for, or simulate, certain actual processes within the aquatic environment. This excludes models that are only statistical relations between dependent variables, blackbox models that ignore internal dynamics, and models that simulate internal dynamics by unrealistic formulations that are not, or cannot, be measured. These more mechanistic models must follow the same standard procedures of model development, calibration, and verification as have the simpler models; however, as will be discussed below, additional tests may also be necessary to build confidence in application of these models.

The Need for Additional Tests

Often, complete verification of a more mechanistic model is not possible by usual techniques because one does not have a complete and independent data set. This is because sampling all of the properties simulated in more mechanistic models is difficult and expensive (e.g., zooplankton biomass).

Even when a complete verification data set is available and the more mechanistic model has been "verified" by usual techniques, one is left with serious questions concerning reliability for two reasons: 1) calibration and verification tests are subjective and 2) there are increased degrees of freedom in these generally nonlinear models. The first reason will not be discussed here because it is considered elsewhere in these proceedings.

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*GLERL Contribution No. 185

The terms increased degrees of freedom, in this context, means that more than one set of coefficient values will satisfy the usual tests for calibration and verification. The basis for increased degrees of freedom is the cyclic nature of mechanistic models. Since these models generally simulate ecosystem cycles, one would not expect material to accumulate excessively in one particular component but rather to flow among all of the components. Then, because of the principles of mass conservation, one could expect that, if the rate of flow were increased or de creased proportionately, the state variable concentrations would not be affected significantly (at least not within the variability usually inherent in the verification data set).

It is for this reason and because of the lack of long-term data that I am suggesting that additional verification tests be included in the standard procedures for testing mechanistic models.

Two Additional Tests

The first type of test is related to gross dynamics and empirical relationships developed for lakes and is particularly useful when long-term verification data are lacking. The second type of test is related to the verification of internal model dynamics and is useful for reducing the degrees of freedom.

Gross properties--If it is impossible or at least very difficult to verify directly the long-term dynamics of the mechanistic model, one can test it indirectly by comparing model output with output from simpler verified models. An example of this approach can be found in Scavia and Chapra (1977). In this study, the results of a mechanistic model were compared with predictions of annual average total phosphorus made by a simple mass-balance model. The mechanistic model (Figure 1) was run to steady-state under a number of nutrient load conditions. At steady-state, annual average total phosphorus was calculated by aggregating the model components and averaging over a year. For the comparison, a simple steady-state mass-balance model for annual average total phosphorus (Dillon and Rigler, 1974a) was solved with the same nutrient load conditions:

$$P = \frac{L(1 - R)}{q_s}, \qquad (1)$$

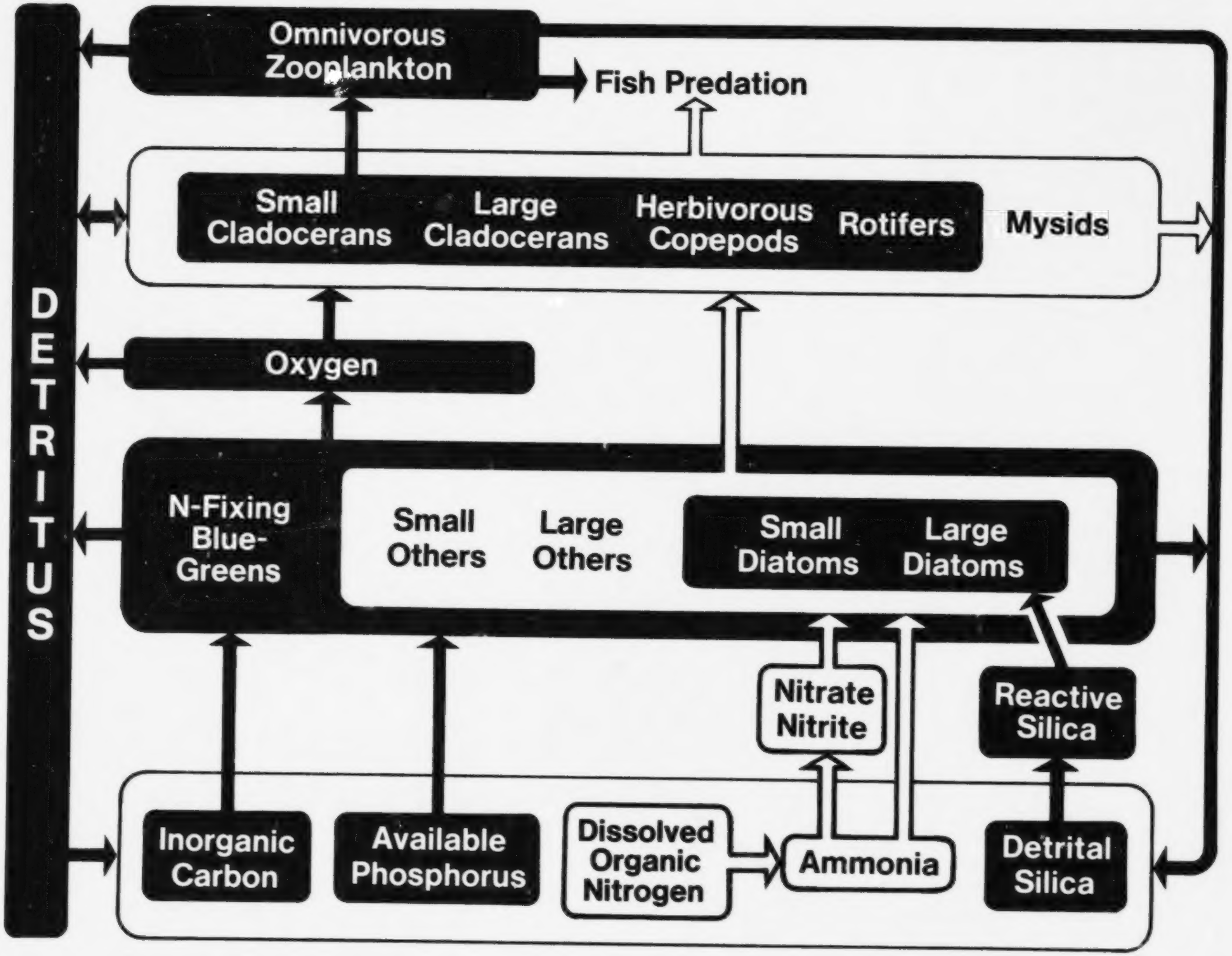

Omnivorous Zooplankton
Fish Predation
Small Cladocerans
Large Cladocerans
Herbivorous Copepods
Rotifers
Mysids
Oxygen
N-Fixing Blue-Greens
Small Others
Large Others
Small Diatoms
Large Diatoms
Nitrate Nitrite
Reactive Silica
Inorganic Carbon
Available Phosphorus
Dissolved Organic Nitrogen
Ammonia
Detrital Silica
DETRITUS

FIGURE I. CONCEPTUAL FRAMEWORK OF MECHANISTIC MODEL

(SCAVIA, 1979a)

where the retention coefficient R is from Chapra (1975):

$$R = \frac{16}{16 + q_s}. \qquad (2)$$

Combining equations (1) and (2) yields:

$$P = \frac{L}{16 + q_s}, \qquad (3)$$

where P = annual average total phosphorus,
L = phosphorus loading rate, and
q_s = areal water load.

The comparison of the results of the two models (Figure 2) indicates that both produce similar estimates of total phosphorus. Therefore, if the mass balance model was a verified model or was proven to be general in most respects, then the mechanistic model could be considered verified to some degree (at least in terms of long-term mass balance considerations).

Scavia and Chapra (1977) also demonstrated another way to test a mechanistic model in terms of gross properties. In this test, the model output was treated like lake data to see if it conforms to an empirical correlation known to be applicable for a wide variety of lakes. In other words, the model was tested to see if it was behaving like the lake. The correlation (Dillon and Rigler, 1974b) relates ($r = 0.95$) summer average chlorophyll 'a' (chla) to spring total phosphorus (Pv) for a data set of 46 lakes, each with a nitrogen to phosphorus ratio greater than 12:

$$\log_{10}[\text{chla}] = 1.449 \log_{10}[\text{Pv}] - 1.136. \qquad (4)$$

It is reasonable to assume that equation (4) represents well a large cross section of lakes. For model comparison, the mechanistic model (Figure 1) was run under a number of conditions, and for each year that $N{:}P>12$, spring total P concentrations and summer average chlorophyll 'a' concentrations were calculated. These results were then plotted (Figure 3), along with equation (4). The agreement between model output and the empirical curve was good up to a point. Beyond about 75 μgP/l, the model output diverged consistently from the line. Thus, in this case, confidence in the model was inspired because it reproduced the relationship between spring phosphorus and summer chlorophyll 'a'; however, other important information was also obtained. The model failed to function consistently under extremely eutrophic conditions. Scavia and Chapra (1977) suggest causes for the failure, but the important point here is that

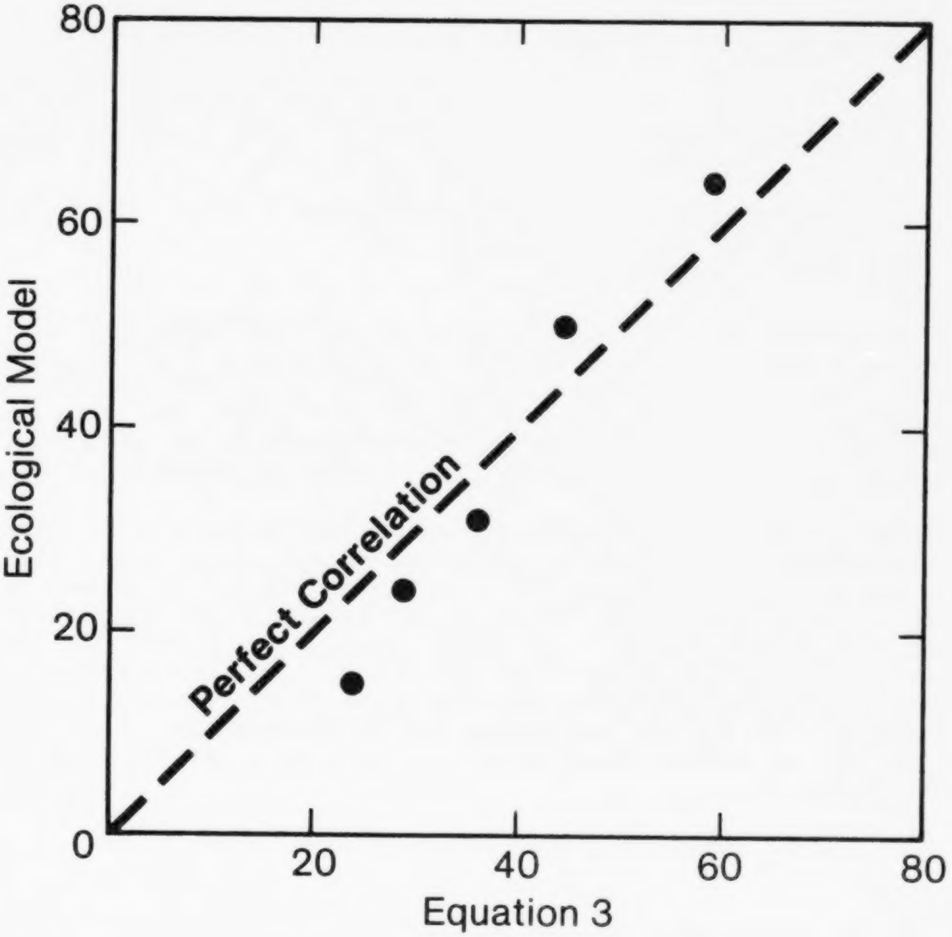


FIGURE 2. COMPARISON OF TOTAL PHOSPHORUS CONCENTRATION (mg/m^3) AS CALCULATED BY THE MECHANISTIC MODEL AND BY EQUATION (3)

(SCAVIA AND CHAPRA, 1977)

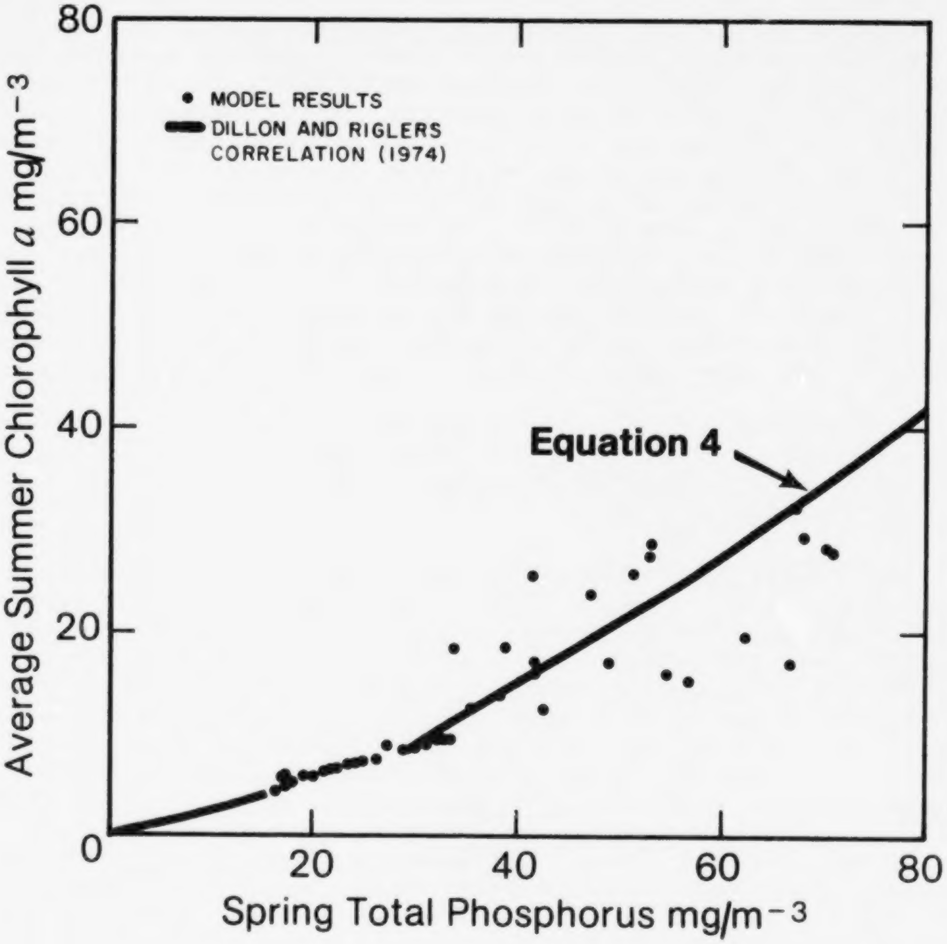


FIGURE 3. COMPARISON OF MECHANISTIC MODEL RESULTS AND CORRELATION LINE BETWEEN AVERAGE SUMMER CHLOROPHYLL a AND SPRING TOTAL PHOSPHORUS

(SCAVIA AND CHAPRA, 1977)

this verification procedure provided a test of confidence as well as set a possible limit to the model's applicability.

Internal dynamics--The second type of verification test proposed here is verification of the internal dynamics of the mechanistic model. One of the most important reasons for using mechanistic models is to examine the controls of the system. For example, a mechanistic model can be used to examine the controls of phytoplankton production (Figure 4) and phosphorus cycling (Figure 5). In this context, model output is used to estimate the timing and relative magnitude of the influence of specific processes on state-variable dynamics. One important question concerning this use of the model is whether the simulated process rates are accurate representations of real processes. As mentioned above, compensating errors at the process level might lead to a successful calibration at the state-variable level. Thus, if models are to be used at the process level and we are to have faith in the dynamics that produce the state-variables, we must look closely at the modeled processes.

The following example demonstrates one method of verifying processes and the way in which compensating errors at the process level can lead to erroneous conclusions regarding system controls.

After initial calibration of the state variables in a mechanistic model of Lake Ontario (Figure 1), simulated process rates were compared to actual measurements. For this comparison, a summer averaged (July-Sept.) phosphorus flow diagram was constructed (Figure 6a) from aggregated model output. The flow (or transfer) rates were then compared to measurements and calculations from Lake Ontario and to other, more theoretical estimates. Many of the simulated process rates were very low (as much as 3-7 times lower) compared to actual rates, with the most serious discrepancies in transfers among available phosphorus, phytoplankton, and zooplankton, yet the state variables compared successfully! Therefore, I calibrated the model again, keeping the process rates in mind and most coefficient values still within acceptable ranges. The new calibration is shown in Figure 6b. The interesting point here is that the state variables are close to the originally calibrated values and can still be considered calibrated; however, the process rates are much higher and, in fact, much closer to observed values (Scavia, 1979b).

This example demonstrates that if the model were calibrated only in terms of state variables and then used to examine control of the phosphorus cycle, then the relative importance of certain processes would be overestimated by almost an order of magnitude. For example, bacterial regeneration of available phosphorus (detritus available P) is relatively more important in Figure 6a than in Figure 6b and the relative

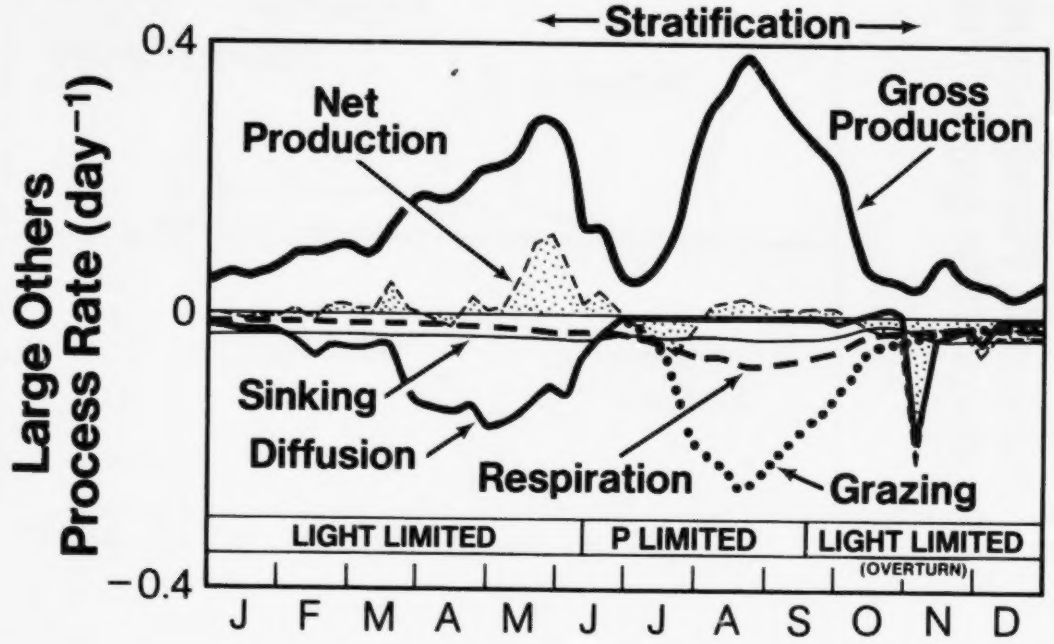


FIGURE 4. RATE PLOT INDICATING SIMULATED CONTROLS OF EPILIMNION PHYTOPLANKTON DYNAMICS IN LAKE ONTARIO

(SCAVIA 1979b)

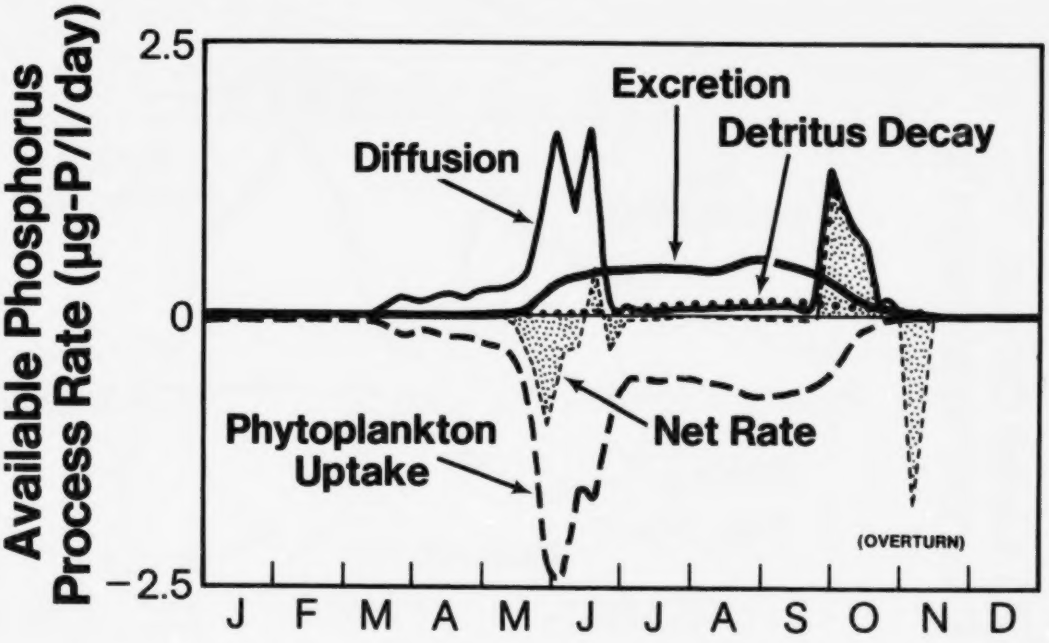
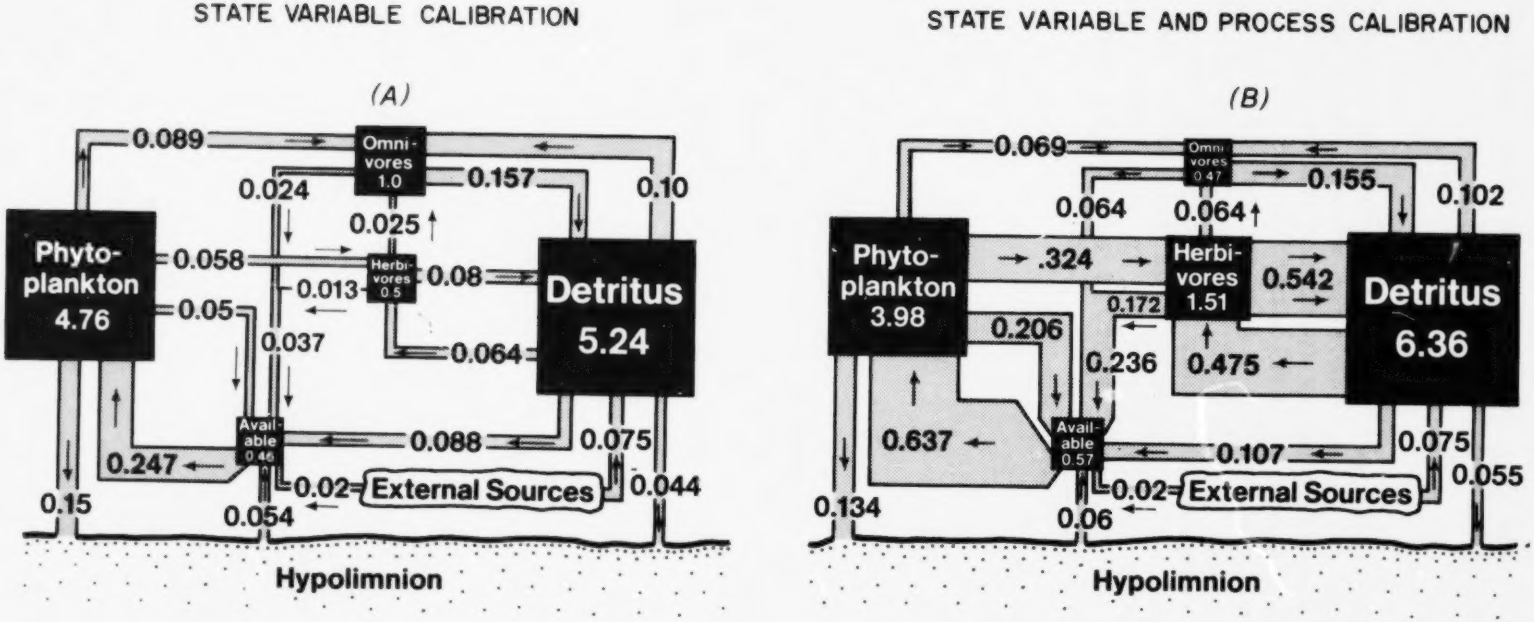


FIGURE 5. RATE PLOT INDICATING CONTROL OF PHOSPHORUS DYNAMICS

(SCAVIA 1979b)



STATE VARIABLE CALIBRATION

(A)

STATE VARIABLE AND PROCESS CALIBRATION

(B)

Phyto-plankton 4.76
Omni-vores 1.0
Herbi-vores 0.5
Detritus 5.24
Avail-able 0.46
External Sources
Hypolimnion
0.089
0.024
0.157
0.10
0.025
0.058
0.013
0.08
0.05
0.037
0.064
0.088
0.075
0.247
0.02
0.044
0.15
0.054
Phyto-plankton 3.98
Omni-vores 0.47
Herbi-vores 1.51
Detritus 6.36
Avail-able 0.57
External Sources
Hypolimnion
0.069
0.064
0.064
0.155
0.102
.324
0.542
0.172
0.206
0.236
0.475
0.637
0.107
0.075
0.02
0.055
0.134
0.06

NOTE:

CONCENTRATIONS IN BOXES ARE IN μg-P/L
CONCENTRATIONS IN PIPES ARE IN μg-P/L/DAY

FIGURE 6. PHOSPHORUS FLOW DIAGRAM

importance of external loads and of transport into and out of the epilimnion is exaggerated in Figure 6a.

Summary

Because of increased degrees of freedom and the usual lack of longterm verification data, mechanistic models need verification tests beyond the standard tests used for state variable simulation. Two general types of verification can be useful additionals to the usual tests: 1) a comparison of aggregated output from the mechanistic model with output from simpler models and empirical correlations that have been verified or proven to be general and 2) a comparison of simulated process rates with rates measured in the field or in the laboratory to determine if the model's internal dynamics are consistent with measured and theoretical dynamics.

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SOME THOUGHTS FOR COMMITTEE BRIEFING - WATER QUALITY & HAZARDOUS SUBSTANCES

MARCH 8, 1979

By

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As I indicated to the program organizers, I am not an expert in either mathematical modeling or in toxic substances in general. I was requested to attend because of my experience with the Hudson River PCB problem.

I have done a considerable amount of work in monitoring dredging activities and have several reports relating to this (1-6). I have also done several years work in collection of sediment samples and in analysis of sediment data for PCB and heavy metals (7,8). In the study of the Hudson River PCB problem, many consultants were retained and studies performed, as noted in Table 1. My work also involved coordinating some of the consultants' efforts, applying their results to develop a solution to a practical problem (PCB in the Hudson River). A summary report on the consultants' results and DEC studies is available (9). Recently, I have become involved in calculations of PCB volatilization from sediments and from water. The volatilization rates of PCB from sediment are high, but can be greatly reduced by capping the sediments with organic topsoil or clay (10,11). There is more information in the above referenced studies than I can possibly describe here. Many of you may already be familiar with the Hudson River PCB problem. If there are any questions on these topics, I will try to answer them.

In the following paragraphs I will mention findings, figures and tables that may be related to modeling of toxic substances, especially PCB, in water bodies in general.

One often learns of toxic substances in water bodies from fish analyses. Fish do biocontrate certain toxics so that their detection is easier. The concentration of toxics in water is often so low that accurate detention and tracing of the source of toxics are difficult. Fish are quite mobile and one cannot

TABLE I. HUDSON RIVER PCB STUDY CONSULTANTS

CONSULTANT OR GROUP	STUDY		STATUS
NORMANDEAU ASSOCIATES BEDFORD, NH	BED SAMPLING AND MAPPING (UPPER HUDSON)		REPORT AND MAPS IN
LAMONT-DOHERTY PALISADES, NY	BED SAMPLING, PCB ANALYSIS, Cs 137 DATING (LOWER HUDSON)		REPORT IN
USGS - ALBANY	RIVER HYDROLOGY WATER PCB AND SUSPENDED LOAD	(1976 & 77) (1978) (1979)	DATA AND PAPERS IN SOME DATA IN
RENSSELAER POLYTECHNIC INST. TROY, NY (DR. T. ZIMMIE)	BEDLOAD SAMPLING (UPPER HUDSON)	(1977)	DATA IN
HYDROSCIENCE WESTWOOD, NJ	PCB MATH MODELING OF UPPER AND LOWER HUDSON	(1977) (1978 - 79)	REPORT IN BEGINNING
LAWLER, MATUSKY & SKELLY ENG. PEARL RIVER, NY	MODELING SEDIMENT AND PCB TRANSPORT AND HYDROLOGY FOR UPPER HUDSON	(NO ACTION) (DREDGING)	REPORT IN BEGINNING
MALCOLM PIRNIE WHITE PLAINS, NY	DREDGING TECHNOLOGY, PLANS, AND ASSOCIATED IMPACTS		7 REPORTS IN
	FINAL PLANS ANS SPECIFICATIONS FOR HOT SPOT DREDGING		TO BEGIN WHEN FUNDED
WESTON INC. WEST CHESTER, PA	PCB LANDFILLS AND DREDGE SPOIL SITES, SAMPLING AND COMPLETE ENVIRONMENTAL ANALYSIS		REPORT IN
O'BRIEN AND GERE ENG. SYRACUSE, NY	1. PCB ANALYSES SEDIMENT AND WATER MEDIA	(1977 - 78)	DATA AND REPORT IN
	2. EFFECT OF PCB ON WATER SUPPLIES (TREATMENT METHODS)		IN PROGRESS
RALTECH (WARF) MADISON, WI	PCB ANALYSES - BIOLOGICAL MEDIA		IN PROGRESS

Table 1, page 2

CONSULTANT OR GROUP	STUDY		STATUS
SYRACUSE RESEARCH CORP.	PCB ANALYSES - SEDIMENT AND WATER MEDIA		BEGINNING
NYS DEC BUREAU OF AIR RESOURCES	PCB AIR SAMPLING	(1977 - 78)	DATA IN
NYS DEC BUREAU OF FISH AND WILDLIFE	FISH DATA ANALYSIS	(1977 - 78)	IN PROGRESS
NYS DEPT. OF HEALTH	MACROINVERTEBRATE ANALYSIS, HEAVY METALS ANALYSIS, LAB QUALITY CONTROL, SOME PCB ANALYSIS, Cs 137 DATING		IN PROGRESS
GENERAL ELECTRIC CORP., RES. & DEV. SCHENECTADY, NY	SEDIMENT INCINERATION, PCB VOLATILIZATION, PCB BIOLOGICAL DEGRADATION, NON-DREDGING PCB RENOVATION OPTIONS		IN PROGRESS WAITING FINAL REPORT
	ENVIRONMENTAL EFFECTS OF PCB SUBSTITUTE-DIELECTROL I, II		REPORT IN
	TOXICITY OF PETROLEUM HYDROCARBONS		BEGINNING
BOYCE THOMPSON ITHACA, NY	SAMPLING VEGETATION AND LAND IN FT. EDWARD TO ALBANY AREA		BEGINNING
FORDHAM UNIVERSITY NYU MEDICAL CENTER SUNY, STONY BROOK, NY	BIOLOGICAL SAMPLING, LABORATORY MODELING AND PROJECTIONS FOR LOWER HUDSON		BEGINNING
*MT. SINAI SCHOOL OF MEDICINE NEW YORK, NY	HEALTH EFFECTS OF GENERAL ELECTRIC FACTORY WORKERS		WAITING FINAL REPORT
CORNELL UNIVERSITY AND AGRICULTURE AND MARKETS ITHACA, NY	ANALYSIS OF CROP AND FOOD DATA		PLANNED

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* Not funded by DEC.

accurately locate the sources and sinks of the problems by fish either. Sediments are much less mobile and are one of the best medias to analyze for toxics. Toxic compounds such as PCB are stored in the sediments at concentrations of 10^3-10^5 times the concentrations found in water. It would seem that a vital input needed to most water models of toxics would be good sediment data.

For the upper Hudson it was concluded the sediment PCB values were log normally distributed. In some low velocity areas near the bank, PCB concentrations of 900 μg/g were found, as noted in Figure 1. In the main channel of the river, the sediment was often sandy and much lower in PCB (15-20 μg/g). The downriver variations (Figure 2) in PCB concentration were much more gradual than the across river variations. In the Hudson one could find two or three samples in a mucky, near bank area 20 miles downstream of the source of PCB averaging 300 μg/g, while an area 2 miles downstream of the source of PCB in the center of the channel in sandy sediment, the PCB may average only 15 ppm. If one preceeded on the philosophy that he should simply average all the PCB samples at a given river mile to obtain the average river bed concentration, one could wrongly conclude that the PCB was 20 times as high 20 miles downriver as it was 2 miles downriver from the source of PCB. The solution is to divide the river into different types of areas on the basis of velocity, depth, sediment texture, and presence of emergent vegetation, and then average the PCB concentrations in those respective areas.

Another factor to consider is the partitioning coefficient between the PCB in sediment and the PCB soluble in water. Table 2 gives some of the experimental values. The method of defining solubility is difficult. In an elutriate test, a lot of colloidal solids are suspended that are difficult to separate from the water and the exposure of the sediment is increased over its exposure in a river situation. The strength of binding of the PCB to different sediment types is also a factor as noted in Figure 3. As the organic carbon content of the sediment increases, PCB is more tightly bound (12). Other factors affecting partitioning coefficients are described in several references (13-17).

1. The specific PCB isomer and position of chlorine attachment.
2. The ionic strength of the water (PCB is less soluble in salt water than in distilled water).
3. The method of defining solubility.
4. The conditions of mixing in the test.
5. The concentration levels of PCB used.

Another topic of concern is the transfer of PCB from sediment to water by erosion (bedload and suspended load).

TABLE 2. SEDIMENT TO WATER PCB PARTITIONING COEFFICIENTS

TYPE STUDY	AROCLOR	COEFF.*	AUTHOR
SEDIMENT MIXED AND SETTLED	1242,1016	1.3×10^3	(16) PARIS ET AL. (1978)
MIXED AND SETTLED	1254	6×10^4	(---) HALTER AND JOHNSON (1977)
WATER FLOWS OVER SEDIMENT IN TANK	1254	9×10^5	(---) HALTER AND JOHNSON (1977)
MIXED AND SETTLED (ELUTRIATE)	70% (1016)	10^3-10^4	(---) LMS-GE,HUDSON RIVER (1976)
FLOW OVER IN TANK	70% (1016)	$10^{4\#}$	(---) LMS-GE,HUDSON RIVER (1976)
MIXED AND SETTLED	70% (1016)	10^3-10^4	(1) TOFFLEMIRE (1976)
MIXED AND SETTLED	70% (1221)	10^3	(1) TOFFLEMIRE (1976)
FLOW OVER TANK	80% (1016)	2×10^5	(--) VEITH,HUDSON RIVER (1976)
ELUTRIATE TESTS, HUDSON RIVER	70% (1016)	10^3-10^4	(--) NYS DEPT. OF TRANS. (1976-7).
MIXED AND SETTLED FOR 5 CITIES IN U.S.	70% (1254)	10^3-10^4	(--) FULK ET AL. (1975)
MIXED AND SETTLED	70% (1016)	10^4	(18) GENERAL ELEC.,MCFARLAND (1977-8)
ELUTRIATE TESTS $\frac{1}{10}$, $\frac{1}{10,000}$	70% (1016)	$10^3, 3\times10^4$	(--) MALCOLM PIRNIE (1977)

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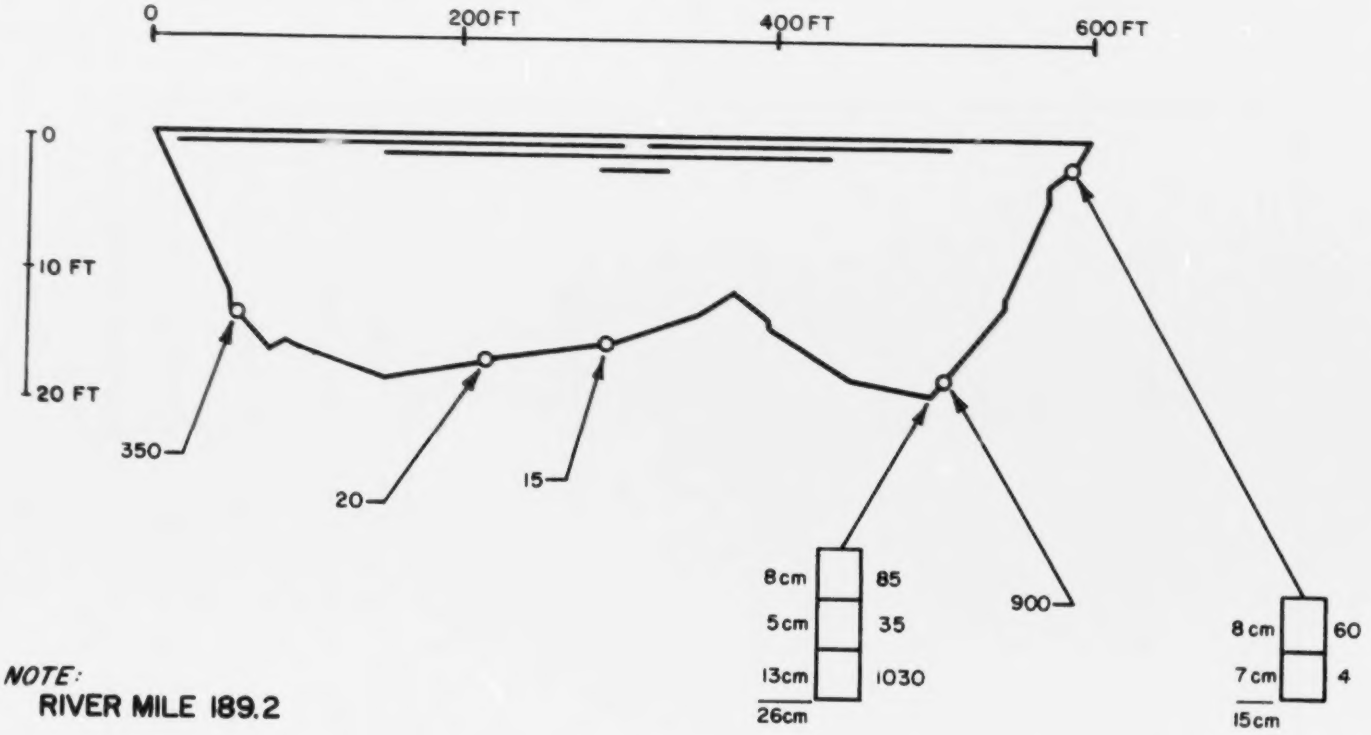
[*] Dry sediment conc./soluble water conc. (.45μ filter or centrifuge).

[#] Here there was 200 mg/l of suspended solids in the water tested.

	1221	1016 & 1242	1254
ELUTRIATE DREDGING SIMULATION	10^3	5×10^3	2.5×10^4
FLOW OVER IN TANK - RIVER SIMULATION	2×10^4	10^5	5×10^5



0
200 FT
400 FT
600 FT
0
10 FT
20 FT
350
20
15
900
8 cm
5 cm
13 cm
26cm
85
35
1030
8 cm
7 cm
15cm
60
4

NOTE:
RIVER MILE 189.2

FIGURE I. PCB CONCENTRATIONS IN BED MATERIAL

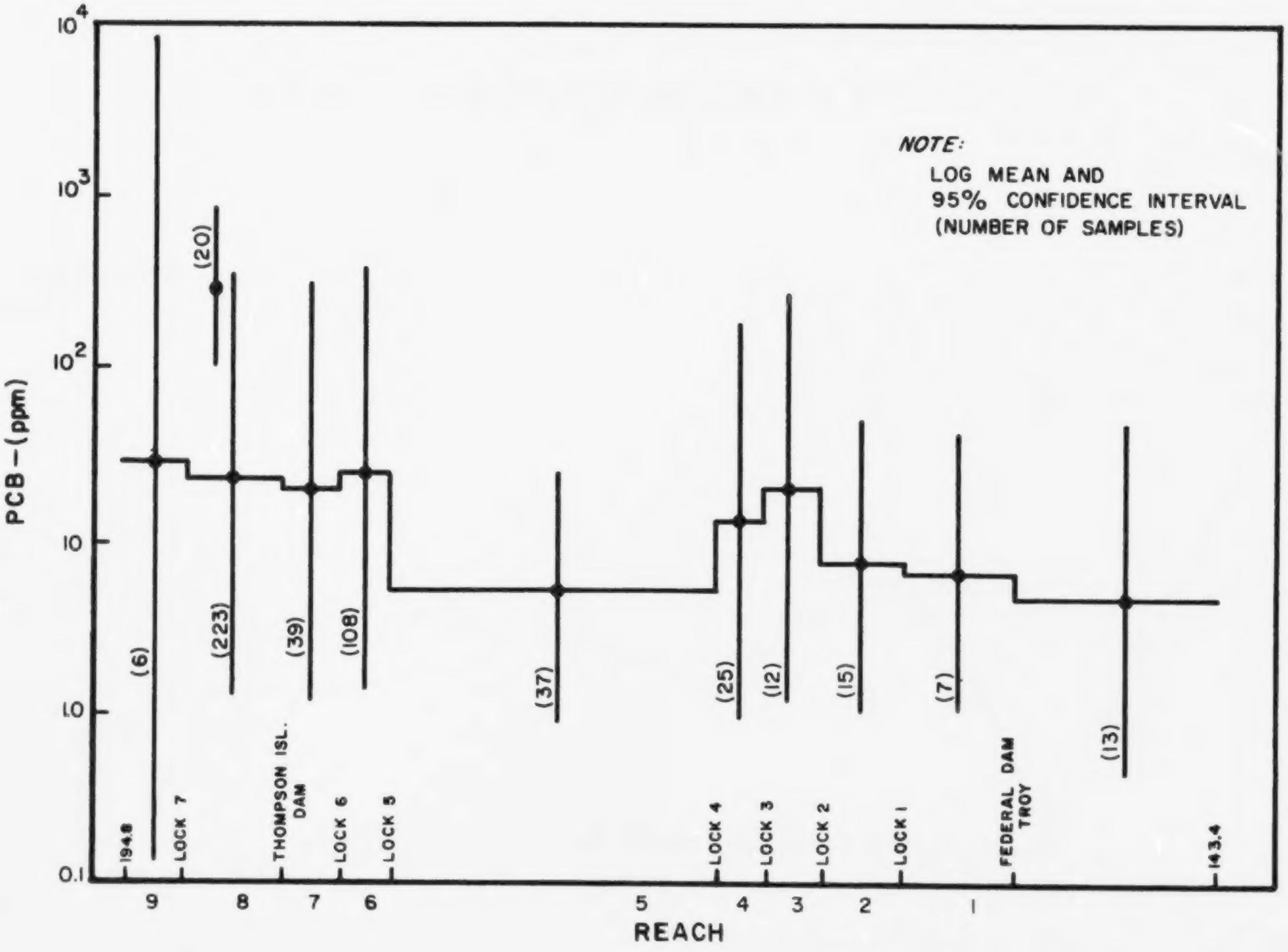


FIGURE 2. AVERAGE PCB CONCENTRATIONS IN SEDIMENTS OF HUDSON RIVER

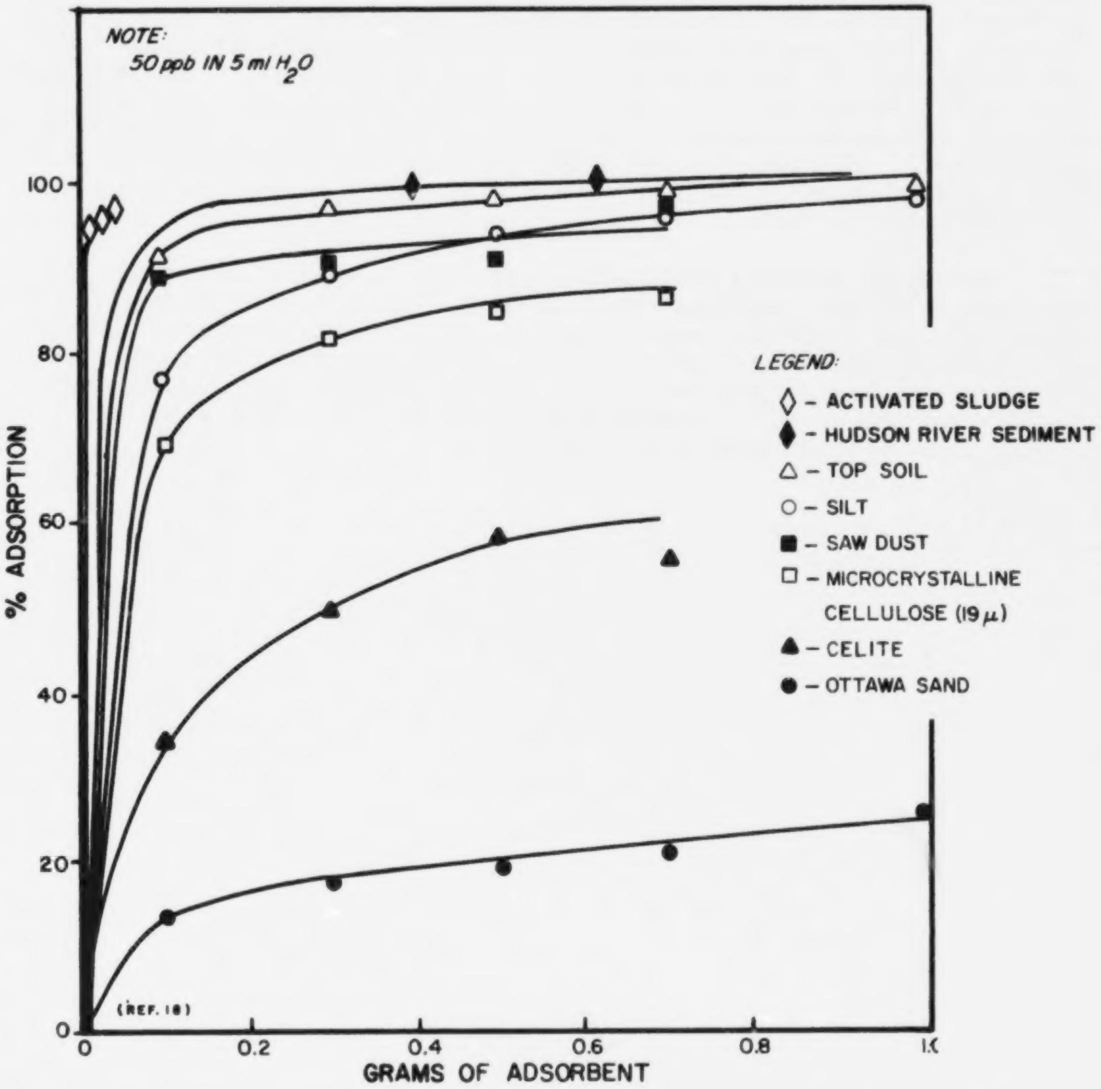


FIGURE 3. ADSORPTION OF AROCLOR 1242 ON DIFFERENT ADSORBENTS

Models are available to predict erosion of non-cohesive sediments (sands) that need little experimental calibration. Models to predict erosion of cohesive sediment (silt and clay deposits, marshes, etc.) require considerable experimental studies for calibration. In the Hudson it is the cohesive organic sediments that are highest in PCB. A practical problem, such as suspension of PCB-laden sediment by barge traffic, may also have to be considered. Figure 4 shows that the PCB concentration in the river water is high at low flow and at very high flows but low at intermediate flows.

PCB also volatilizes quite rapidly from the water to the air and from the sediment to the air. Figures 5 and 6 give plots of experimental data from GE (18), while Figure 7 gives approximate estimates of transfer rates and mass storage figures. Table 3 compares some of the literature values for volatilization. All references given in the table were not listed in the attached bibliography.

TABLE 3. COMPARISON OF K VALUES FOR VOLATILIZATION OF PCB AT 25°C

For PCB Saturated Water

Aroclor	Mol. Wt.	Solubility μg/ℓ	Vapor Pressure mm Hg	KCs mg/m²/hr	KCs pure PCB μg/m²/hr	$\bar{K}$ 1/hr	$\bar{K}/\bar{K}_2$
1221	192	(1000)[a] (1000-2000)[e]	≈ (10^{-2})[e]	(.055-.090)[a]	$(3.3\times10^{+3})$[a]	(.002-.004)[a]	
1242	261	240 (80)[e], (340)[d]	4.1×10^{-4} (9×10^{-4})[e], (3×10^{-4})[d]	13.7 (1.8-5.0)[b]		.057, (.002-.006)[a] (.2-.9)[d], (.0096-.027)[b]	(.22)[d]
1016		(175+)[a], (420)[d]	(2×10^{-4})[d]	(.009-.016)[a]		(.3-1.2)[d]	(.25)[d]
1254	321	12 (56)[c]	7.7×10^{-5}	.8	$(8.35\times10^{+3})$[c]	.067	

Reference (--) Mackay and Leinonen was used unless otherwise noted.
(a) GE-Corp. Res. Niskayuna, NY - Brooks et al. (18)
(b) GE-Corp. Res. Niskayuna, NY - McFarland, et al. (18)
(c) Hague, et al. (17)
(d) Paris, et al. (16)
(e) Huntzinger, et al. (--)

For Sediment or Soil to Air Transfer

Aroclor	Soil PCB μg/g	KC μg/m²/hr	Air Conc. ng/m³	half life in top 10 cm - yrs	Area or Soils	Reference
1254	.01	1.25	1-10	6	LaJalla, Calif.	(--) McClure
1254	10			.1	Ottawa Sand	(17) Hague, et al.
80%(1016)	64.	126	1200	<.1	Sand & Wood Chips	(18) G.E., McFarland
80%(1016)	20		100		Sand & Wood Chips	(--) DEC-Air Resources
1248	.04		10		Lake Michigan Area	(--) Versar Inc.
1242, 1254	.05			<.05	Sand	(18) GE, Brooks
1242, 1254	.05			>.3	Silt or Top Soil	(18) GE, Brooks

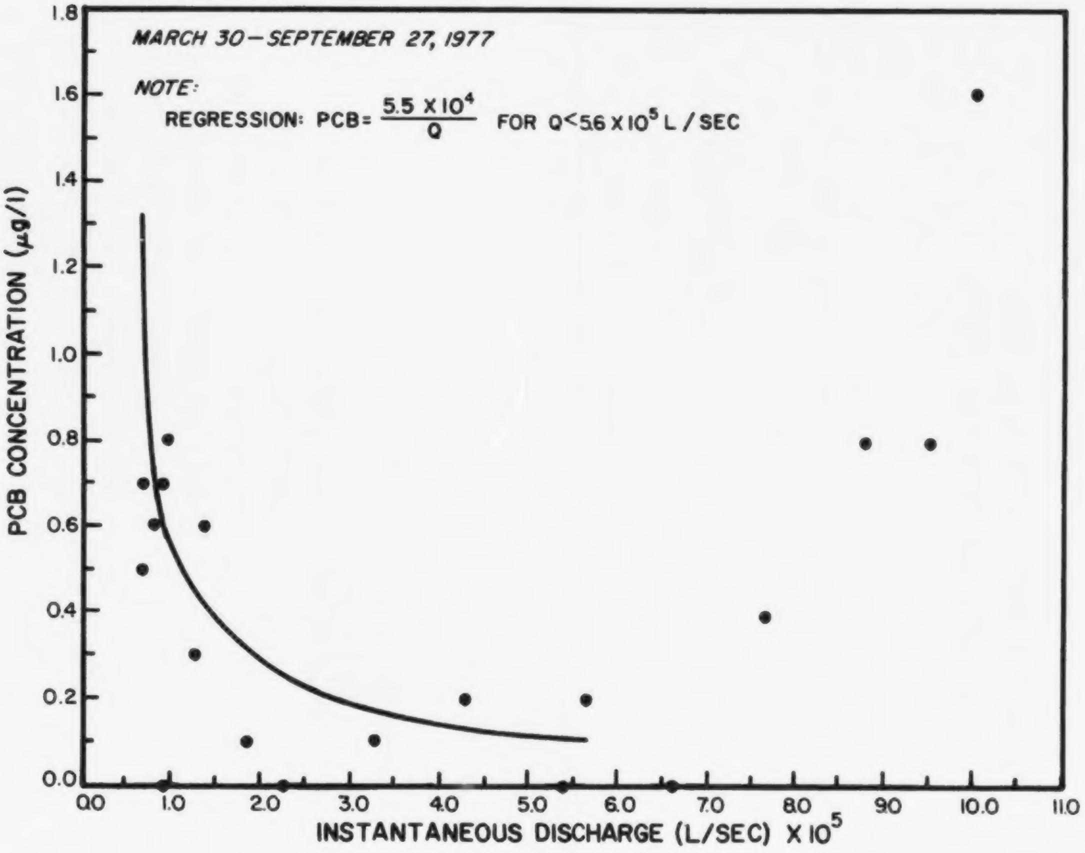


FIGURE 4. HUDSON RIVER AT SCHUYLERVILLE
PCB CONCENTRATION VS. RIVER DISCHARGE

SOURCE: TURK, USGS DATA

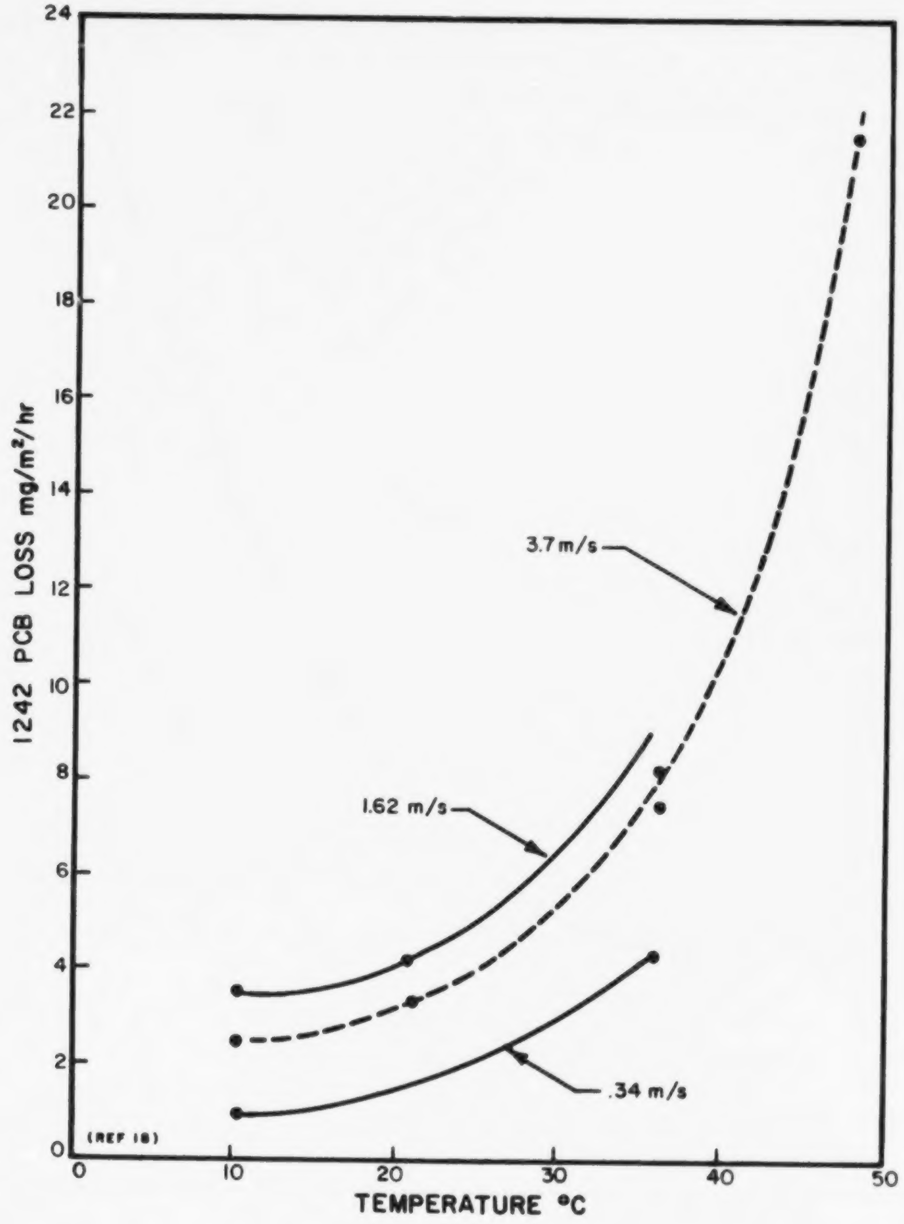


FIGURE 5. PCB LOSS FOR 1242 SATURATED WATER

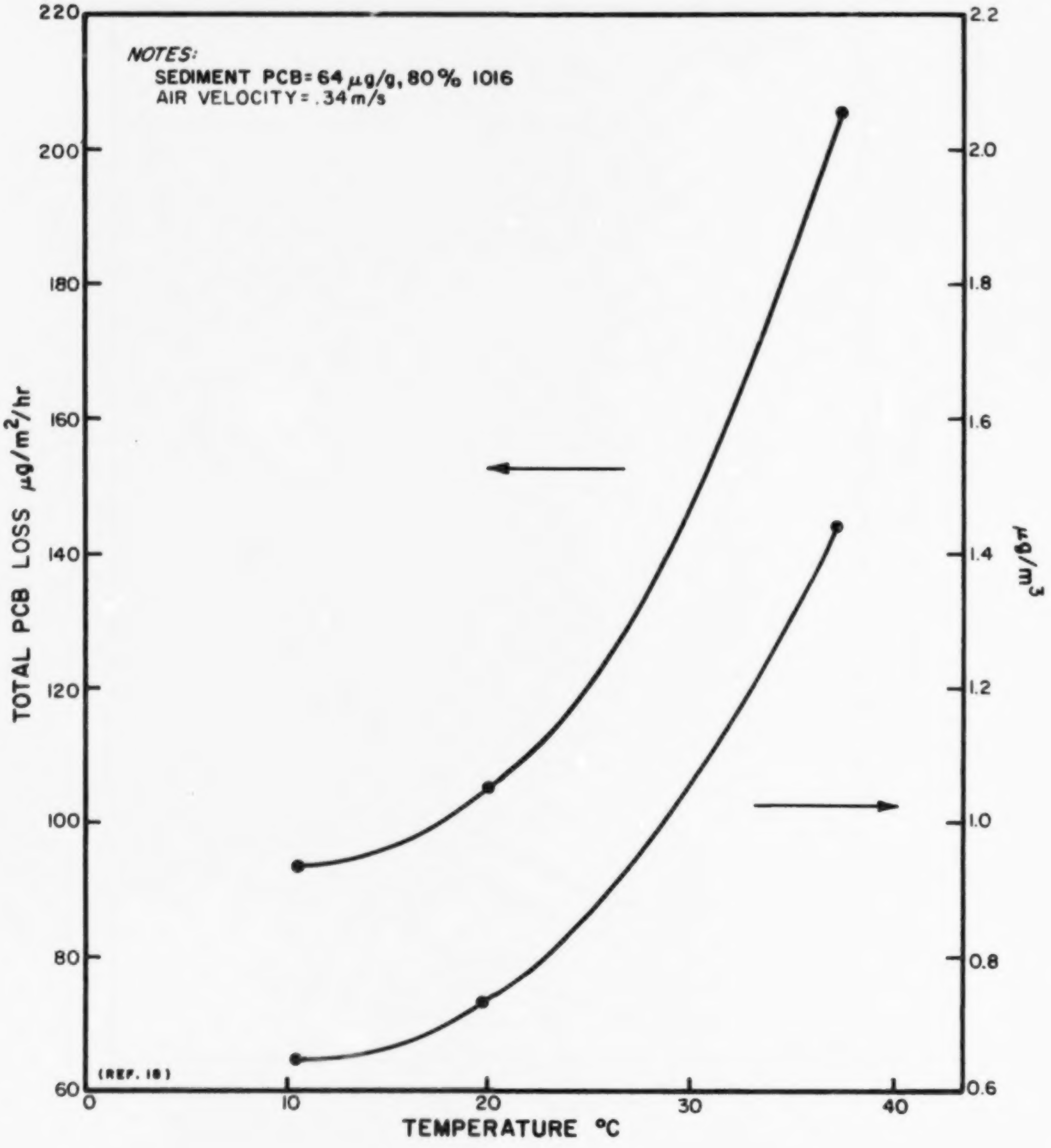
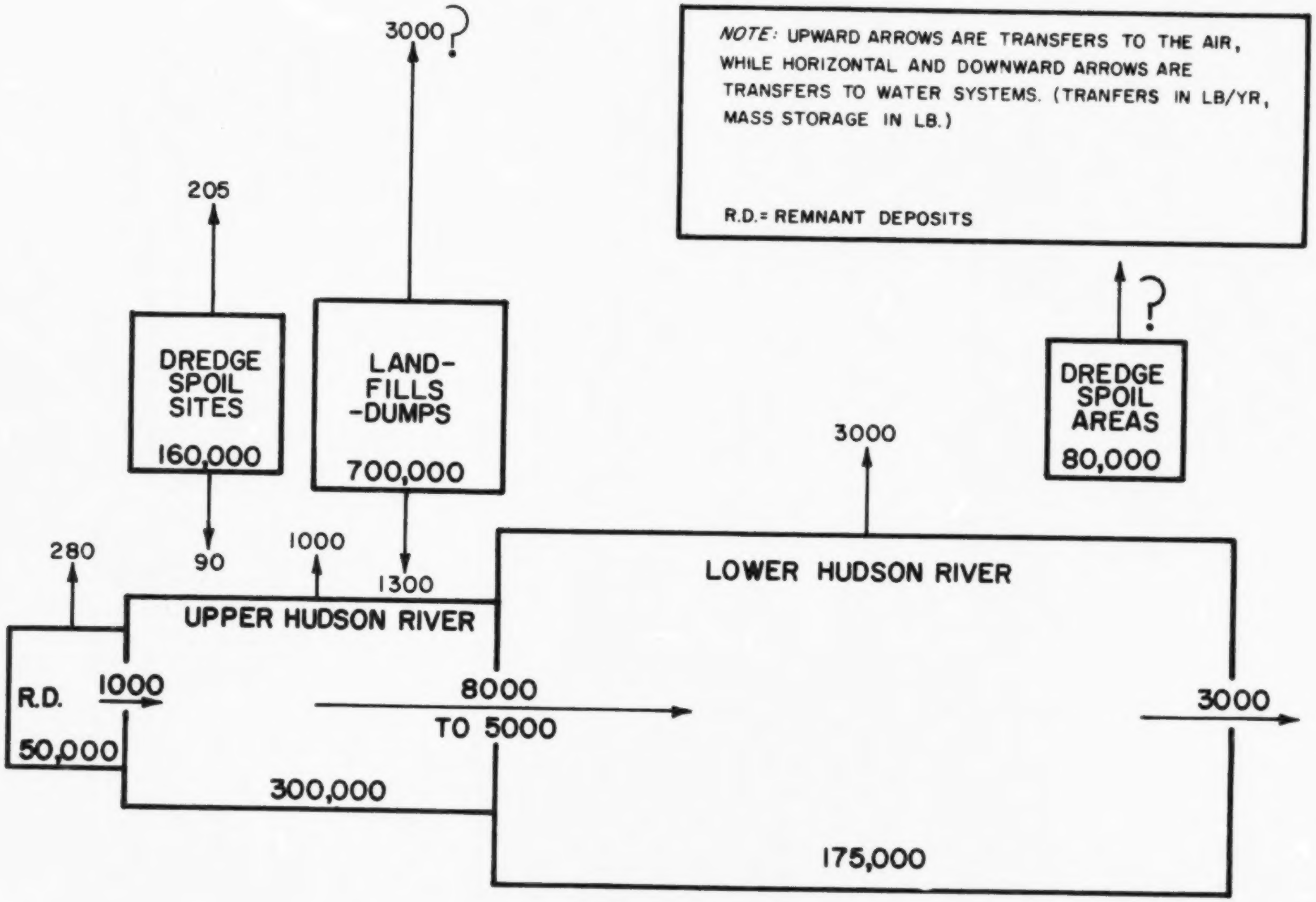


FIGURE 6. SEDIMENT TO AIR PCB LOSS


3000?
205
DREDGE SPOIL SITES
160,000
LAND-FILLS -DUMPS
700,000
DREDGE SPOIL AREAS
80,000
?
3000
280
90
1000
1300
R.D.
50,000
1000
UPPER HUDSON RIVER
300,000
8000
TO 5000
LOWER HUDSON RIVER
175,000
3000

NOTE: UPWARD ARROWS ARE TRANSFERS TO THE AIR, WHILE HORIZONTAL AND DOWNWARD ARROWS ARE TRANSFERS TO WATER SYSTEMS. (TRANFERS IN LB/YR, MASS STORAGE IN LB.)

R.D.= REMNANT DEPOSITS

FIGURE 7. DISTRIBUTION AND TRANSFER OF PCB IN THE HUDSON RIVER BASIN AS OF JANUARY, 1979

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WORKSHOP ON VERIFICATION OF WATER QUALITY MODELS, DISCUSSION PAPER, WASTELOAD GENERATION

By

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The generally poor ability of deterministic models to adequately predict the rates of pollutant accumulation, transport and transformation prior to arrival in a receiving water body is, in my estimation, our most serious modeling problem. There are those who would argue that receiving water quality models are in even worse shape and should hence receive priority attention. I firmly believe, however, that until we are reasonably able to predict loadings, or are able to be more specific about how unable we are to make these predictions, our efforts must be concentrated in this area.

The most commonly cited reason for the sad state of these models is a lack of suitable data for their calibration and verification. It is certainly true that the data base is woefully small, and that those in possession of such data are frequently reluctant to share their knowledge. This has forced the users of these models into having to collect large amounts of data on each individual project in order to assure themselves that model results are "accurate" (whatever that means).

It is my opinion, however, that attention should be concentrated on the model formulations themselves. Loading models are, for the most part, predicated on fitting an equation or equations to a limited amount of data then using other data to calibrate such a model to fit local conditions. Seldom have enough data been used, or have these data been subjected to a rigorous enough analysis to assure that the loading function postulated is indeed the "correct" one. Little work has been done in examining the formulations themselves, in order to determine whether or not they actually describe physical processes taking place.

Such examination would seem to be the purview of the research community, yet those folks seem extremely reluctant to tackle the problem. I suspect that one reason for this is that such research is not very satisfying, and is quite difficult. Another reason, certainly, is that agencies who sponsor such research have, by their failure to budget for much work of this sort, in effect said that the problem has a relatively low priority.

The problem, however, will not go away. I am sure that those of you who are consultants (and your clients) have, at times, been uneasy about the "accuracy" of modeling results. We are, moreover, increasingly moving toward making environmental decisions based on receiving water quality rather than on effluent quality. A good example is the rigorous evaluation of receiving water impacts now required for AWT projects. We are also moving, I believe, toward the establishment of water quality standards which reflect the stochastic nature of such bodies. Given this emphasis, it is not enough to concentrate on better water quality models. However elegant they may be, they are driven by imperfect loading models which limit the validity of our modeling results. It seems incumbent on all of us, therefore, to try to straighten the mess out.

I believe that there are several things we can do. First, and most important, we can all be more generous about sharing catchment data that we have. One way of doing this is to put data into a commonly-held data base, such as the urban data base at the University of Florida, or STORET. Second, we can take upon ourselves a more critical examination of the quality formulations in our loading models. We have, in the past, based model comparisons on overall evaluation of model performace, and not on examinations of various model components, such as pollutant accumulation/washoff functions. Third, we can publish results of such examinations so that others may benefit from our experience. I devote a good portion of my time to technology transfer activities, and I am convienced that no one suffers as a result of telling others exactly what he is doing. It is manifestly clear that there is plenty of work for everyone!

DISSOLVED OXYGEN/TEMPERATURE MODELING

By

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Our assignment is to discuss DO/Temp. modeling in the context of the six "Issues" raised. Although my emphasis shall be on DO, much of what I have to say applies equally to temperature modeling. I suggest we consider each of these issues under current status and shortcomings, and suggested recommendations.

Issue #1 - The Role of Models in Decision Making

At the outset, let us face it, modeling as it has more recently developed is not generally accepted by administrators as a usable tool. In fact, modeling in general today has not only gained a bad reputation, but is regarded with considerable mistrust. As EPA no doubt can verify, most current models are gathering dust on the shelves of "computer software libraries". We might ask what is wrong with current practice? There is too much "sophistication"; too much complex math; too much talking of modelers with each other, rather than with administrators; failure to present modeling results for ease of user understanding; and most important, the frequency of failure of models to hook up in application to a real-river case.

The proliferation and promotion of the theoretical-general-case model as a tool for practical application should be discouraged; such models should be confined to research and academic training. Concentration should be on development of practical-applied models specific for each particular river, oriented to its unique problems and basin conditions. Mathematical complexity should be avoided, with the accent on simplification and ease of understanding of the administrator.

Issue #2 - Data Base

"Date Base" - for what purpose? If by data base the purpose is to accumulate, on a national scale, vast amounts of "monitoring" data upon which it is expected that reliable water-quality models can be developed, we are deluding ourselves and wasting taxpayers' money on a costly, inefficient, unreliable endeavor. Unfortunately, the current trend is strongly toward collecting more and more "monitoring-type data". Monitoring is not designed to obtain adequate data under hydrologic nor biologic stability, conditions so essential to reliable measurement. Rather, monitoring obtains data under all kinds of changing conditions, and hence represents a heterogeneous mess, much of which is useless. Furthermore, monitoring is seldom correlated with waste loadings and hydrologic conditions. Hence, monitoring data reflect effect without simultaneous measure of cause, and therefore give little or no insight into cause-effect relationships.

However, there are two types of long-term records available, namely, hydrologic and meteorologic data, that are important but are seldom adequately analyzed. These data identify the critical season in which water quality occurs, and afford the means of defining recurrence probability to which model predictions must be related. One would expect that these findings would be used in the design of the stream sampling program and in the selection of model configuration, but they usually are not.

Water-quality monitoring data should be restricted and limited to their primary role as an administrative tool in surveillance in routine regulatory practice, not as a tool in planning, design, and decision making, and certainly not in development of reliable predictive models. The concept of accumulation of a "data base" for water-quality modeling should be discouraged. Successful river-quality assessment and modeling require fresh, new, concurrent data. Such data can be obtained only through carefully planned intensive, synoptic-type river-quality investigation. This necessity has long been recognized, and has been more recently demonstrated, with dramatic results, in the USGS reports of the applications in the Willamette and Chattahoochee Rivers. It is urged that, instead of worrying over "data base" details, a fundamental change in approach should center on establishing, on a continuing basis, a National Intensive River-Quality Assessment Program for all major river basins.

Issue #3 - Model Configuration

There is a misconception that because seasonal changes in water quality occur, it is essential to formulate a dynamic model to simulate instantaneous responses throughout the year. This necessitates a Eulerian configuration of exceedingly complex mathematics and requires extensive data, not realistically attainable from stream and laboratory measurements. In the end, "assumptions" are necessary both in parameters and in solutions of the complex math. The net result is much confusion, loss of model reliability and false economy in time and cost.

The Eulerian frame of the general-case-dynamic model configuration should be supplanted by the Lagrangian configuration of the applied-steady-state model. This eliminates the complex mathematics without loss of scientific validity. The river, based on channel geometry, is segmented into short reaches, and only simple computations are necessary on a segment-by-segment basis.

It is well established that the critical water quality period almost invariably occurs annually during the drought season low streamflow and high temperature. A steady-state period of 2-3 weeks usually occurs each year uninterrupted by freshets, in which hydrologic and biologic equilibrium are approached, ideal for intensive stream sampling and concomitant measurement. It is noteworthy that, unlike the Eulerian, in the Lagrangian configuration parameters are all relatively easily and accurately derived from stream measurements, without any "assumptions". And since intensive parameter measurements need be made only for the steady-state condition, the economy in time and cost is obvious.

Issue #4 - Calibration

In calibration one observes three phases of dangerous degeneration taking place:

Phase I--failure to obtain adequate current data. Modeling is not a function independent of intensive analysis of the river system, yet fewer and fewer modelers get into the field to become intimately familiar with the river and to participate in the gathering of current concomitant data necessary for analyzing cause-effect relationships.

Phase II--overuse of existing data. Most modelers are content to use existing old, monitoring-type data. Some recognize the deficiencies and try to augment by averaging composites of seasonal data over the years of record; this is like "averaging early peas with late pumpkins".

Phase III--overuse of mathematical and computer techniques. Other modelers, particularly mathematicians and computer specialists with little real river experience, resort to "optimization" to quantify model parameters (usually obtained from scanning the literature, not from field investigation). Then by multiple regression techniques a "best fit" is obtained, which is taken as the "optimum" value. Seldom is the "optimum" value checked for validity within the river system being modeled. This type of calibration must be regarded as little more than sophisticated "curve-fitting", and the reaction rates thus generated are highly suspect. In contrast, there is a tendency of some modelers to concentrate exclusively on refinements of theory in calibration, most of which prove to be insignificant relative to the recurrence probability frame of the immediate hydrologic and meteorologic variations of the specific river basin.

The use of monitoring data for calibration for river-quality modeling should be discouraged. Calibration should be based on current concomitant data obtained from intensive field sampling and investigation (under hydrologic and biologic equilibrium) on the specific river being modeled. Obviously, each reaction rate, (BOD, nitrification, reaeration, etc.,) should be independently calibrated on its own relevant data.

Issue #5 - Verification and Sensitivity Analysis

The current trend to attempt application of models without verification is shocking! It is no wonder that such models are increasingly distrusted. In other cases verification and calibration are based on the same set of data, usually poor data at that. In some instances where reasonably good calibration and independent verification have been made, seldom are limits specified within which application of the model is feasible. There is also a misconception that once a good applied model has been calibrated and verified, it can be used indefinitely, even though radical changes in river conditions have taken place over the years.

Models which have never been adequately calibrated and verified should not be promoted for application in evaluation of alternatives in water-quality management. It is a disservice to modeling and to society to do so. Good verification implies comparison between two independent sets of data, one for calibration of reaction rates, and a new second set for verification. If there is reasonably good agreement between the computed and the observed river quality, the verification is accepted, and application of the model for predictive evaluation of still other conditions (within limits prescribed) is then, and only then, warranted. Models cannot be used indefinitely, regardless of how carefully calibrated and verified initially. Intensive reassessments should be made at intervals of 5-10 years or so for re-calibration and re-validation. Such reassessments also afford the only reliable measure of achievement attained by remedial programs instituted. Hence, the most rigorous test of reliability is demonstration of agreement between actual achievement and what the projection predicted would occur. Furthermore, the consistency with which this can be demonstrated, when the method of analysis (or modeling) is applied to other river systems, is the best way to build confidence in use and acceptance of the method.

As a supplement to verification, sensitivity analyses should be made for each element calibrated. The sensitivity analyses are good indicators, where review of the calibration should be made for refinement.

Issue #6 - Use of Models as Projection Tools

Again, the single greatest stumbling block to the use of models as projection tools is failure to develop practical-applied models, carefully calibrated and verified from good data, for each specific river for which projections are desired. Since all projections of river quality are inescapably tied to probability of occurrence of hydrologic and meteorologic variability, much too little attention is given to establishment of a frame of reference in which practical decisions must be made concerning recurrence expected, such as once in 5, 10 or 20 years.

Quite apart from development of the model, practical projection implies that an intensive investigation in depth be made of the river basin as a whole, its problems, plans, and proposals. Useful projections cannot be made in a vacuum. In addition, there is increasing need for sharp scrutiny and evaluation of the consequences of imposition wholesale of arbitrary water quality standards.

Unfortunately, there are groups in and out of Government laboring under the delusion that there must be some easy, quick or magic way for computers and modeling to project wholesale answers to all water-quality problems. There is no easy short cut, and modeling should not be oversold. There is no substitute for careful thought and intensive investigation in the search for cause-effect relationships river-by-river, tempered by intimate experience and professional judgment--the art and science of river analysis.

SALINITY/TDS:
APPRAISAL OF PRESENT PRACTICES AND CAPABILITIES IN MODELING

By

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1. Salinity and total dissolved solids are virtually conservative parameters within the interior of natural waterbodies.

    1.1 Waste discharges involving high TDS, e.g. brine disposal from oil wells, represent point sources and are generally modeled as such, not as an internal generation rate. (An exception is an oil field distributed over a section of a large waterbody.)

    1.2 In those models involving a depth mean, i.e. two-dimensional horizontal models or section-mean models, the net evaporation-evaporation minus precipitation-at the surface represents an effective source (sink) when positive (negative). This source function is mathematically first-order, a rate constant multiplying the salinity.

        1.2.1 Inclusion of the evaporative source of salinity is rarely important, except in shallow systems located where the evaporative deficit is significantly different from zero, i.e., in arid or in wet-humid climates.

2. Accordingly, the distribution of salinity or TDS within a waterbody is determined primarily by the boundary fluxes and the internal transport processes within the system.

    2.1 Transport processes are traditionally subdivided into advective versus diffusive (turbulent) transports. However, various spatial and temporal averages applied to the basic equations of mass transport produce cross-product terms which themselves must be parameterized. This parameterization most frequently has the form of a diffusive flux, whereupon the transport is termed "dispersion". As transport processes are discussed elsewhere, their further consideration in this context is not warranted.

2.1.1 Because of their virtually conservative character and their natural occurrence, especially in estuaries, salinity and TDS enjoy an importance in the calibration of various water quality transport models. Thus the need for a capability to model salinity extends beyond the parameter *per se*.

2.2 One important boundary source for salinity/TDS is the flux from the bed and sides of a waterbody, derived ultimately from geological sources. This is common in watersheds that drain areas of extensive salt domes or areas in which the principal aquifers are in contact with salt domes.

2.2.1 An interesting example is Lake Texoma on the Red River on the border between Oklahoma and Texas. TDS values in this lake are on the order of 1000 ppm and range up to values double this below the halocline.

2.3 Longitudinal fluxes of salinity/TDS are important to waterbodies in hydrodynamic contact with a more saline system. The most common and important example of this is, of course, the estuary.

2.4 Because salinity distribution within a waterbody is determined by transport, with practically no internal kinetics, the time scales upon which salinity reacts to an alteration in the boundary fluxes is generally much longer than time scales for, say, dissolved oxygen or nitrogen species.

2.4.1 In many cases, the dissolved oxygen profile within a stream, say, is determined principally by the rates of oxygen supplied by reaeration versus the rate of oxygen utilization deriving from the introduction of organics into the watercourse. The effect of transport is to modify the net rate slightly, producing a displacement and, perhaps, spreading of the dissolved oxygen profile. In contrast, salinity distribution is determined solely by the various transport processes, to which the isohaline pattern must readjust.

3. A practically unique feature of salinity/TDS, vis-a-vis other common water quality parameters, is its interaction with density, frequently dominating the effects of temperature and dictating the density structure of the waterbody.

   3.1 Vertical gradients in salinity substantively suppress vertical turbulent fluxes of mass and momentum. (Further discussion of this factor should be undertaken as a part of transport mechanisms.)

   3.2 Longitudinal gradients in salinity produce a horizontal pressure-gradient acceleration that can drive density currents, which can be a prominent element of the overall circulation of the waterbody.

   3.3 The single most important and common example of salinity-induced density currents is in estuarine circulation.

      3.3.1 Estuarine density currents manifest themselves as systematic vertical and/or horizontal shears in the current. These currents are persistent in time, independent of tidal phase, and are quintessential in the long-term mean circulation and constituent distribution in the estuary.

      3.3.2 For a given longitudinal salinity gradient, the intensity and spatial structure of the density current are a strong function of bathymetry. In estuaries with a prominent longitudinal geometry and little cross-channel relief, the density current produces two-layered mean flow, up the estuary toward the head in the lower layer compensated by flow down the estuary toward the mouth in the upper layer. In estuaries that are broad with a central talweg, the mean flow is directed up the talweg channel throughout the depth, compensated by a seaward return flow in the shallow lateral areas to either side.

   3.4 Rigorous modeling of salinity and transport when density effects are important requires a coupling of the momentum and salinity calculations.

      3.4.1 The common practice for estuaries, however, is to avoid this difficulty by parameterizing the density current transport by inflated dispersion coefficients in the salinity model. This converts the momentum-salinity model from a feedback (i.e., interactive) problem to a feedforward problem.

3.4.2 The dispersion coefficients are determined by forcing a match of mode output to observations, model calibration. The resultant coefficients are employed in other salinity computations (e.g. different inflows) as well as in the transport of other constituents such as DO. This has become accepted through practice, not theory.

3.4.3 Physical models include density transport implictly, but only qualitatively, not quantitatively, in that (so long as water is the model fluid) the dynamic scaling (Froude) is not sufficient to ensure similitude (which would also require-at least-Reynolds similitude). There is, therefore, a calibration procedure for these models as well, resulting in the establishment of a set of bent strips, cobbles, overhead fans and even forced-air diffusers.

3.4.4 Whatever justification there may be for extending model application beyond its range of calibration, it is manifest from 3.3.2 above that this calibration is invalidated when bathymetry is altered.

4. Verification of models of salinity or TDS is complicated by the slow response times of these parameters.

4.1 The problem of response time is particularly acute in estuaries, which tend to be large waterbodies with substantial salinity gradients impressed over their entirety.

4.1.1 Tests with the San Francisco Bay physical model and simulations with the EPA Dynamic Estuary Model indicate the response time-constant of salinity to a 30,000 cfs freshet was 8 tidal cycles at Carquinez Strait and 15 tidal cycles at Point San Pablo. Termination of the 30,000 cfs pulse and immediate (step function) reduction back to the 2,000-3,000 cfs low flow indicated a decay time-constant of 8 tidal cycles at Point San Pablo and 10 tidal cycles at Caruinez Strait.

4.1.2 Within the Galveston Bay System, salinity variations in East Bay following a reduction in inflow from 20,000 cfs to 1,000 cfs indicated a time-constant of approximately two months (or 60 tidal cycles). East Bay is generally the last segment of the system to equilibrate, and it is speculated that a more realistic time-constant for the entire system is on the order of 30 tidal cycles.

4.2 The long response time for the salinity/TDS distribution within the system affects the verification procedures as well as the accuracy of verification for both steady-state and time-dependent models.

4.2.1 For steady-state model verification, the basic assumption is that the isohaline distribution has equilibrated to the freshwater inflows. This requires two conditions: stabilization of the freshwater inflows at a specific value (of course, within a certain tolerance, since small fluctuations are integrated out); elapsing of enough time-constants for salinity response to ensure the isohaline structure has equilibrated.

4.2.2 As a rule of thumb, two to three time-constants are necessary to ensure equilibration. This requires, in turn, that the freshwater inflows be stabilized for this period. From the results indicated in 3.1 above, a period of one to several months of steady inflows are necessary. It is important to recognize that time equilibration of the inflows is necessary but not sufficient for time equilibration of the isohalines.

4.2.3 A time-varying model is the solution to an initial-boundary problem, in which the initial salinity distribution is an important input. This is generally determined from observations. Transient variations in freshwater inflow result in transient departures of salinity from this initial value, but significantly filtered by the long response time for salinity. This means that short periods of time integration produce minor departures from the initial conditions, and hence apparently good verification against measured data. A long period of integration, rather, is required to determine whether the basic model is seriously in error in its ability to predict salinity.

4.2.4 An illustration of the time increase in error of a dynamic salinity model is the operation of the Galveston Bay physical model for salinity with 1965 hydrological inputs. For the first five months of model simulation, the model results were still dominated by the initial conditions and compared very well with measurements. For the sixth month and thereafter, the model predictions departed markedly from measurements, being systematically low on the order of 5-10 ppt.

5. Perhaps because of the difficulty of securing satisfactory data sets for either time-dependent or steady-state verification, verification of salinity/TDS models is often pursued through a statistical approach utilizing a steady-state model.

5.1 This is based upon the postulate that a steady-state (i.e., time-equilibrium) solution with long-term mean inflows and boundary conditions will somehow approximate the long-term mean salinity.

5.1.1 There is absolutely no theoretical justification for this postulate. Indeed, the intrinsic nonlinearity of the transport equation for salinity would render such a postulate unlikely.

5.2 Some sort of empirical verification of this postulate is required. Clearly verification of an equilibrium model in this respect constitutes a *de facto* validation of the postulate. It is, however, a site-specific validation only.

5.2.1 To this writer's knowledge, a sufficiently detailed and statistically rigorous validation of the "climatological" capability of steady-state models has never been performed. Again, though such a validation would be useful, it must nonetheless be site-specific.

5.2.2 One of the difficulties in this regard is the necessity for a long term data base on salinity, sufficiently refined in time to permit calculation of means *and* their statistics, from which confidence bounds can be established.

6. Recommendations (of this writer) for improvement of the state-of-the-art in modeling of salinity are improved hydrodynamic formulation of the transport terms and an introduction of methodological rigor in model verification.

   6.1 Better hydrodynamic foundation for the density effects of salinity upon transport is needed. For estuaries, in particular, the longitudinal transport ("dispersion") is a significant weakness of present models. This will require theoretical studies coupled with intensive, carefully specified data collection.

   6.2 More attention is needed to quantify the quality of model prediction with respect to confidence limits of the data. Proper data stratification taking into account salinity response time is necessary.

   6.3 For the broader questions of model verification in general, this writer suggests that our discipline has much to learn from the experiences of the meteorologists.

      6.3.1 There are several analogues between our problems and those of the meteorologists. We both deal with large scale fluid systems, that exhibit variability on a range of space time scales. Numerical models of hydrodynamics and transport are an essential element in the analytical procedure for both fields. The adequacy of predictions are tested by comparison with quantitative fluid parameters, sparsely distributed in time and space.

      6.3.2 Practicing meteorologists employ several models, and combine the results of these models with judgment (founded upon their experience with the processes involved as well as with the behavior of the models) to arrive at a prediction. Much of this judgment, it should be noted, is site-specific. This role of judgment is frequently denigrated in our discipline and sought to be replaced by-rather than supported by--the operation of models, whereas it should be cultivated.

      6.3.3 Meteorologists are faced with the problem of verification on a daily basis. Some of the statistics they have devised to evaluate performance are, of course, of interest to the water-quality disciplines. More to the point, though, is the verification of model behavior not so readily parameterized, such as movement or intensity of features of the hydrodynamic field.

6.3.4 Verification, in the meteorological field, is a convergent judgment, based upon the cumulation of many individual predictions. In the water quality discipline, in contrast, verification frequently consists of a single data set compared with the corresponding model prediction, a practice which ignores the stochastic elementin the measured data as well as the departure of the physical configuration from that assumed in the model formulation. Perhaps the most important aspect of the introduction of statistical measures in water quality model verification, whatever these measures might be, is the implication of testing the model against an array of data sets.